

Introducing Groups into Quantum Theory (1926 – 1930)

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Abstract

In the second half of the 1920s, physicists and mathematicians introduced group theoretic methods into the recently invented “new” quantum mechanics. Group representations turned out to be a highly useful tool in spectroscopy and in giving quantum mechanical explanations of chemical bonds. H. Weyl explored the possibilities of a group theoretic approach towards quantization. In his second version of a gauge theory for electromagnetism, he even started to build a bridge between quantum theoretic symmetries and differential geometry. Until the early 1930s, an active group of young quantum physicists and mathematicians contributed to this new challenging field. But around the turn to the 1930s, opposition against the new methods in physics grew. This article focusses on the work of those physicists and mathematicians who introduced group theoretic methods into quantum physics.

Introduction

In the middle of the 1920s, understanding of the representations of Lie groups and understanding of the quantum mechanical structure of matter made great advances, almost simultaneously. Certain members of both disciplines saw the potential for building new and deep connections between mathematics and theoretical physics. Thus a cooperative development highly consequential for theoretical physics began in the second half of the 1920s, with the main protagonists being W. Heisenberg, E. Wigner, F. London, W. Heitler and, to a lesser degree, P.A.M. Dirac on the one side, H. Weyl, J. von Neumann, and B.L. van der Waerden on the other. The first introduction and use of the new method in theoretical physics met soon with opposition (“group pest”). But it turned out to be successful in the long run, and to be just the first wave of a process of restructuring mathematical concepts and techniques in the theory of the basic structures of matter. After an intermediate period of about two decades with a slow and nearly unnoticed continuation of work in this direction, another wave of using group-theoretical methods in physics gained momentum in the second half of the century. This development has recently attracted interest from the side of history and philosophy of science.¹ It should be quite as interesting from the point of view of the history of mathematics, because it established broad and consequential semantical relations for an important field of modern mathematics.

¹(Mehra/Rechenberg 2000/2001, Gavroglu/Simóes 1994, Karachalios 2003, Brading 2003)

The following article explores the first wave of introduction of new mathematical methods into quantum physics and chemistry. It starts with the early realization of the usefulness of group theoretic methods for the study of spectroscopy and chemical bonds, and stops short of the consolidation of what was achieved in the first wave in three textbooks on the subject published in the early 1930s, (Weyl 1928, ²1931), (Wigner 1931) and (van der Waerden 1932), which have now become classics of the field. Unlike the other two, Weyl's book had an earlier first edition at the end of the 1920. It therefore enters the period of investigation of our investigation.

This article is a first step into this interdisciplinary terrain from the side of history of mathematics. It relies heavily on the solid background laid out by T. Hawkins' study (Hawkins 2000) and H. Rechenberg's chapter on group theory and quantum mechanics in (Mehra/Rechenberg 2000/2001, VI 1, chaps. III.4, III.5).

1. Heisenberg and Wigner

Shortly after the invention of the new quantum mechanics, P.A.M. Dirac, W. Heisenberg, and E. Wigner started to consider consequences of symmetry in multi-particle systems for the structure of energy terms in atomic spectra.² Dirac studied the role of antisymmetry in multi-electron systems in summer 1926. Important as that was for the growing understanding of quantum mechanics, it did not employ group theory beyond the distinction of the signum of permutations. Group theoretic questions proper started to be addressed by Heisenberg and Wigner in late 1926 and early 1927.

The newly established paradigm of quantum mechanics demanded to characterize a (quantum) physical system, at the time typically an electron system in the shell of an atom or of a molecule, by a set of Hermitian (or more generally, symmetric) operators, one for any observable quantity of the system, in a state space \mathcal{S} assumed to be a Hilberts space in order to have sufficient symbolical structure. In Schrödinger's perspective, \mathcal{S} was viewed as a space of complex "wave" functions. Then the tool of differential operators could be used.³ Most important was the operator characterizing the energy of the system (or a constitutive part of it, like an electron in a multiparticle

²For the emergence of matrix, wave, and "q-number" mechanics see, among others, (Hendry 1984, Beller 1999, Pais 1986, Rechenberg 1995, Cassidy 1992, Kragh 1990, Moore 1994). A multi-volume encyclopedic report is (Mehra/Rechenberg 1982–2001, vols, II, III, IV, V). A six-page compression of the crucial period 1923 – 1926 can be found in the introduction to volume VI (Mehra/Rechenberg 2000/2001, VI 1, xxv–xxx). For a splendid bibliography see (Mehra/Rechenberg 2000/2001, VI 2, 1253–1439); indexes of the whole series at the end of the same volume VI 2.

³Questions how the function space was to be completed, or how domains of the operators should be understood and, perhaps, extended, were generously neglected by the early quantum physicists. Such questions were first addressed by J. von Neumann in the later 1920s and at the turn to the 1930s.

system), the *Hamilton operator* H . Other operators could characterize linear momenta P_i or coordinatized spatial positions Q_i ($1 \leq i \leq 3$), rotational (orbital) momenta L_i , the square of the total momentum L^2 , and, a little later, the *spin* J of a particle (considered to express the “particle’s” proper rotation) etc..

For an atom, the eigenspaces of the Hamilton operator H could characterize the stationary states of a system of electrons, or of an outward electron, depending on the situation. The eigenvalues E_1, E_2, \dots of H represented the energy values obtained in these states. Often such eigenstates turned out to be degenerate, i.e., they belonged to an eigenvalue of multiplicity > 1 . This was the case for atoms or molecules with rotational symmetry. Of course, spectroscopy did not allow to measure the energy of each eigenstate directly. Only differences between two energy values, say E_1 and E_2 , were observable by the frequency ν of the radiation emitted during the transition of an electron from one energy state to the other,

$$h\nu = E_1 - E_2 .$$

In early 1925, Pauli conjectured that bound electron states in a molecule have an intrinsic two-valuedness and that electrons obey an *exclusion principle* forbidding different electrons (a littler later also other “fermions”) to occupy the same state of a system. Later in the year, S. Goudsmit and E. Uhlenbeck established the hypothesis of electron *spin* which they assumed to arise from a “proper rotation” of the electron. Different empirical evidence indicated that this intrinsic spin was quantized with respect to any specified spatial direction in exactly two possible states u and d (spin “up” and spin “down”). Early in 1927, W. Pauli mathematized the idea by a spin state space \mathbb{C}^2 extending the complex phase of the Schrödinger wave function $\psi(x)$ (Pauli 1927). In group theoretic language, which was not yet in Pauli’s mind in early 1927, he implicitly worked inside the natural representation of SU_2 , the covering group of the spatial rotations SO_3 . He proposed to describe a spinning particle by a two valued wave function $\tilde{\psi} = (\psi_1, \psi_2)$, later called a *Pauli spinor*.⁴ It could be constructed from Schrödinger wave functions by forming (tensor) products with the complex two-dimensional space characterizing the complex superpositions of the two possible pure spin states $\mathbb{C}^2 \cong \langle u, d \rangle$ (here $\langle \rangle$ denotes the linear span). The total wave function of a collection of n electrons was expressed formally as a “product” (in later terminology as an element of the n -fold tensor product $\bigotimes^n \mathcal{S}$). In summer 1926 P.A.M. Dirac realized that Pauli’s exclusion principle implied that multi-electron (more generally fermion) states had to be represented by

⁴Pauli drew upon the symbolic ressources of the Klein-Sommerfeld theory of the spinning top, which contained the natural representation of SU_3 implicitly. For a review of the understanding of the rise of spin see (van der Waerden 1960) or (Mehra/Rechenberg 1982, chap. VI.4).

alternating products (Dirac 1926).⁵

An ad-hoc usage of permutations (W. Heisenberg)

Already before Pauli's mathematization of spin was known, Heisenberg started to consider the consequences of the new phenomenon for multi-electron systems. In June 1926 he submitted his first paper on this topic to *Zeitschrift für Physik* (Heisenberg 1926). He looked for reasons for the separation of energy terms in the spectrum of higher atoms into different subsets between which apparently no exchange of electrons took place (*term systems without intercombination*). Such an effect could be seen by "missing" lines when one compared the observed spectral lines with the combinatorics of all the arising energy levels in a higher atom. Heisenberg guessed that the interaction of the orbital magnetic momentum of electrons (i.e., the magnetic momentum resulting from what was left from Bohr's electron orbits in the new quantum mechanics) with the still hypothetical spin might play a crucial role for this phenomenon (Heisenberg 1926).

In a second part of the paper, submitted in December 1926, he continued to explore the hypothesis further. He proposed the view that the distinction of term systems might result from a kind of "resonance phenomenon" between the spin states of the different electrons and, perhaps, their orbital momenta. He made clear that here the word "resonance" was not to be understood in the sense of classical physics, but as an expression of a physical intuition of the "more subtle interplay of the electrons in an atom" (Heisenberg 1927, 556, 578). Thus Heisenberg's "quantum mechanical resonances" referred to spin coupling effects for which at that time no adequate mathematical representation was known.⁶ He therefore looked for new tools to deal with them and hoped to find them in the theory of permutation groups.

In his investigation, Heisenberg studied states of n -electron systems in an atom or molecule. Abstracting at first from spin, he started from n eigenfunctions l, m, \dots, p (Heisenberg's notation) of the Hamilton operator, which described possible states of single electrons without spin, possible degeneracies included. As usual he described a composite system by a kind of noncommutative product of the eigenfunctions. He considered the result as a state of the "unperturbed" composite system, while the spin coupling ("resonance") had to be taken into account as a perturbation due to the "more subtle interplay of the electrons". Because electrons are indistinguishable, he concluded:

In the unperturbed case, the eigenfunction of the total system can be written as product of all functions of the single electrons,

⁵Cf. (Kragh 1990)

⁶In early quantum chemistry the term "resonance" was used in a comparable metaphorical way; see (Mosini 2000).

e.g., $l_1 m_2 \dots p_n$. The unperturbed problem is $n!$ -fold degenerate, because a permutation of the electrons leads to equal energy values of the total system. (Heisenberg 1927, 557)

For an element u of the (tensor) product space, written by our author as $u = l_1 m_2 \dots p_n$ with an index $1 \leq i \leq n$ for the different electrons, Heisenberg considered the result of an electron permutation $S \in \mathcal{S}_n$, the symmetric group of n elements, and wrote it as

$$Su = l_{S(1)} m_{S(2)} \dots p_{S(n)}.$$

If we denote the state space of a single electron by $V = \langle l, m, \dots, p \rangle$, $\dim V = n$, the ($n!$ -fold degenerate) total state space of the quotation above corresponds to the span of vectors arising from permutation of the components of any one product state u .⁷ We want to denote it here as $V^{(n)}$

$$V^{(n)} := \langle Su \mid S \in \mathcal{S}_n \rangle \subset \otimes^n V.$$

$V^{(n)}$ was constructed to characterize the state space of an “unperturbed” system of n electrons distributed according to Pauli’s principle (i.e., mapped bijectively) on the n states m, l, \dots, p . Without spin the energy was totally degenerate (all eigenvalues identical), while the consideration of spin split it up into different “non-combining” terms. The physical model of the electron system had to account for the impossibility of transitions of electrons between the respective states or subspaces. Mathematically the question was whether the corresponding vectors (wave functions) or subspaces in Hilbert space were orthogonal.

Heisenberg looked for a decomposition of $V^{(n)}$ into “noncombining” (orthogonal) subsystems if spin resonance was considered as a kind of perturbation. As we will see in a moment, he had good arguments that orthogonality of subspaces should not be affected by the spin perturbation. Its basic structure could thus be analyzed already on the level of the unperturbed system without spin.

In order to address this question, Heisenberg considered a cyclic subgroup of \mathcal{S}_n generated by a “substitution” (permutation) S of highest possible order

⁷We may prefer to distinguish Heisenberg’s basic state vectors by a lower index i , $\psi_1 = l, \psi_2 = m, \dots, \psi_n = p$, and to characterize the bijection between states and electrons by adding an upper index j , $\psi_i^{(j)}$ ($1 \leq i, j \leq n$). Then it is advisable to order the tensor product according to electron indexes, $\psi_{i_1}^{(1)} \otimes \psi_{i_2}^{(2)} \otimes \dots \otimes \psi_{i_n}^{(n)}$ (comparable to Wigner’s notation, see below). That makes the upper (electron) index redundant, and the lower (state) index i encodes the different possibilities for bijections completely. Because Heisenberg ordered according to states and used the electron indexes to indicate the bijection between electrons and individual states, his permutation S operated on the state vectors of the (“our”) tensor product $V^{(n)}$ by inversion $S^{-1} =: \sigma$, i.e. from the right: $(\psi_1 \otimes \psi_2 \otimes \dots \otimes \psi_n) \cdot \sigma = \psi_{\sigma(1)} \otimes \dots \otimes \psi_{\sigma(n)} = \psi_{S^{-1}(1)} \otimes \dots \otimes \psi_{S^{-1}(n)}$. As this detail has no consequences for the orthogonality questions, we follow Heisenberg’s description in the sequel without further retranslations.

ν , and an orbit in $V^{(n)}$ of an eigenstate u under such a subgroup. He then formed different superpositions of the elements of such an orbit. For a permutation S of order ν he choose coefficients formed by powers of a primitive ν -th root of unity ω , $\omega^\nu = 1$, in the following way:

$$\begin{aligned} U_0 &= \frac{1}{\sqrt{\nu}}(u + Su + S^2u + \dots S^{\nu-1}u) \\ U_1 &= \frac{1}{\sqrt{\nu}}(u + \omega Su + \omega^2 S^2u + \dots \omega^{\nu-1} S^{\nu-1}u) \\ &\dots \\ U_{\nu-1} &= \frac{1}{\sqrt{\nu}}(u + \omega^{\nu-1} Su + \omega^{2(\nu-1)} S^2u + \dots \omega^{(\nu-1)^2} S^{\nu-1}u). \end{aligned}$$

These linear combinations were formed in analogy to the construction of the roots of resolvents in the theory of algebraic equations. In fact, Heisenberg referred to a textbook of higher algebra, a fifty year old German translation of a classical book by Serret (Serret 1868), which had been written originally in 1866 (third edition), as one of the first books containing a passage on the recently revived theory of E. Galois.⁸ For dimensional reasons ($\nu < n!$) there were elements $w = Tu$, $T \in \mathcal{S}_n$, of the defining basis of $V^{(n)}$ (Heisenberg: “eigenfunctions”) which were linearly independent of the $U_0, \dots, U_{\nu-1}$. They lead to analogously formed linear superpositions $W_0, \dots, W_{\nu-1}$. He applied the same procedure, step by step, until the whole space $V^{(n)}$ was spanned by elements of such a form: $U_0, \dots, U_{\nu-1}, W_0, \dots, W_{\nu-1} \dots$ ⁹

Now, Heisenberg collected all functions U_j, W_j, \dots starting with the same exponent j of the unitary root ω into one collection,

$$\Gamma_{\omega^j} := \{U_j, W_j, \dots\},$$

and proposed that the corresponding subspaces could be taken as symbolical representatives for the different term systems. He argued that the span of Γ_{ω^j} and Γ_{ω^k} ought to be orthogonal (for different j and k)

$$\int \bar{f}_j g_k = 0, \quad f_j \in \Gamma_{\omega^j}, \quad g_k \in \Gamma_{\omega^k}, \quad j \neq k. \quad (1)$$

His argument for this claim depended crucially on an invariance argument of the transition integral under any permutation:

If under the integral (...) the electron numbers are somehow permuted, the value of the integral cannot change. (Heisenberg 1927, 559)

The physical context of the calculation demanded such an invariance. Although Heisenberg’s construction of the “term systems” Γ_{ω^j} did not ensure

⁸(Kiernan 1971, 110ff.)

⁹Cf. (Mehra/Rechenberg 2000/2001, 489ff.).

such an invariance, his argument held for similar constructions in which the invariance condition was satisfied.¹⁰ The form of his argument was close to one used in early Galois theory (“as the whole constellation does not depend on the choice of the ordering of the roots of the equation, . . . such and such inference can be drawn . . .”) and may have been prompted by the latter.

Heisenberg agreed with Dirac that an “eigenfunction” of the total system should be antisymmetric under permutation of the electrons. It seemed impossible, at the moment, to draw consequences of this postulate.¹¹ On the other hand, he plausibly assumed that any *perturbation* of transition probabilities, arising from spin coupling, should be symmetric under transposition of two electrons. That was sufficient, in his context, to show that the decomposition of the total space of n electrons $V^{(n)}$ into orthogonal subspaces was not affected by spin resonance. Thus, so he concluded, the subspaces spanned by the Γ_{ω^j} ought to characterize the decompositions of energy terms into non-combining partial systems *including* spin (Heisenberg 1927, 559).¹² Although the argument did not work in his own ad-hoc construction, it would become important (and correct) once it was transferred to a decomposition into truly invariant subspaces.

All in all, Heisenberg’s paper gave an inventive treatment of the term system problem, although it must have appeared surprising for mathematical readers of the time (like J. von Neumann or H. Weyl). For the construction of non-combining term systems, Heisenberg relied on a rather old-fashioned algebraic background (Serret 1868). Neither H. Weber’s textbook (Weber 1895/96) nor any other more recent algebraic text was even mentioned. Such a neglection of more recent methods may not necessarily be of great disadvantage for a new application of mathematics by a physicist. But in this case, the neglection of younger algebraic developments included the methods of representation theory of finite groups, which dealt with structures much closer to Heisenberg’s problem than algebraic equation theory. In his first step into the new terrain, Heisenberg had to rely on formal expressions originally introduced in a completely different context. Thus his hypothesis for the identification of non-combining term systems by his Γ -collections was quite daring and would surely have led to difficulties, had it been used in future investigations without major modifications.

From hindsight it is easy to see that Heisenberg’s decomposition did not lead to irreducible representations of the permutation group. Worse than

¹⁰We will see in a moment (equation (2)) that Heisenberg’s Γ_{ω^j} , respectively their linear spans, are no invariant subspaces under the full permutation group. Heisenberg’s own argument shows that therefore his model was physically unreliable. Wigner’s approach solved the problem. It was different to Heisenberg’s, contrary to what the latter believed.

¹¹A structural answer to this question was given later by Weyl and a more pragmatic one by von Neumann and Wigner, see below.

¹²I thank an anonymous referee for having made me aware of this important passage in Heisenberg’s argument.

that, Heisenberg's hypothetical “non-combining term systems” Γ_{ω^j} were not even invariant subspaces under the full permutation group. His construction made sure that a subspace Γ_{ω^j} is an eigenspace with eigenvalue ω^j of the cyclic subgroup generated by the permutation S . But this does not hold for other permutations. Already for $n = 3$, $\omega = e^{\frac{2\pi i}{3}}$ and any 3-cycle S , e.g. $S = (123)$, a transposition T with $TST = S^2$, e.g. $T = (12)$, maps $U_1 \in \Gamma_\omega$ to $U_2 \in \Gamma_{\omega^2}$,

$$SU_1 = \omega U_1, \quad STU_1 = TS^2U_1 = \omega^2 TU_1. \quad (2)$$

In fact, the linear spans of $\{U_1, U_2\}$ and $\{W_1, W_2\}$, in Heisenberg's notation, are copies of the two-dimensional irreducible representation of S_3 .¹³ In other words, the irreducible spaces are transversal to the subspaces offered by Heisenberg as “non-combining term systems”. But before such discrepancies could start to irritate other contributors to the program, Heisenberg's method was outdated by an approach to the problem proposed by his colleague E. Wigner.

So it was good news, and even better ones than Heisenberg knew, that he could refer to Wigner's investigations already in a footnote added in proof to his December paper. He erroneously believed that his approach agreed with Wigner's (Heisenberg 1927, 561, footnote (1)). In fact, a rash view could support this belief, as in the case of 3-electrons, e.g. a Lithium atom, both methods led to equal numbers and dimensions of the respective term systems: two one-dimensional term systems (symmetric and antisymmetric) and two equivalent two-dimensional term systems (standard representation in Wigner's approach), $6 = 1+1+2+2$. But while Wigner characterized the non-combining term systems by subspaces which actually were irreducible subrepresentations, we have seen that Heisenberg's decomposition was different, even in this case.

In the end, it appears as a lucky sequence of events that Wigner's papers threw new light on the question so fast. His approach superseded Heisenberg's group theoretically ad-hoc method, before the latter could lead into a dead end. Wigner's papers opened the path towards an introduction of group representation into the study of multi-particle systems and established a sound mathematical frame into which Heisenberg's perturbation calculation could be integrated without contradictions.¹⁴

Turn towards group representations (E. Wigner)

Eugene Wigner had studied chemical engineering at Budapest and Berlin (TH) during the years 1920 to 1925 and had gained access to the physical community organized around the colloquia of the *Deutsche Physikalische*

¹³Cf. (Fulton/Harris 1991, 8ff.).

¹⁴In the literature on history of quantum mechanics this essential difference between Heisenberg's and Wigner's approaches is often passed over in silence; cf. e.g., (Mehra/Rechenberg 2000/2001, 489ff.).

Gesellschaft and the local *Kaiser-Wilhelm Institutes*.¹⁵ After he had finished his diploma degree, he went back to Budapest and worked as a chemical engineer in a leather tannery (his father's craft), but he continued to read the *Zeitschrift für Physik* with the interest of an *aficionado*. Thus he was well informed about the breakthroughs in quantum mechanics, achieved during 1925. He immediately accepted the chance to go back to Berlin, when he was invited by Karl Weissenberg to become his assistant at the *Kaiser-Wilhelm Institute* for fibre research. Weissenberg himself had studied applied mathematics with R. von Mises and had then turned towards condensed matter physics. He needed support in his X-ray investigations of crystal structures. At Weissenberg's suggestion, Wigner started to read the group theoretic parts of Weber's textbook (Weber 1895/96) and to explore the symmetry characters of crystals in the new setting.¹⁶ Because of this interest in actual X-ray crystallography, he was much better acquainted with group theory than Heisenberg in 1926.

In late 1926, Wigner started to study the question of how n -particle systems can be built from n given, pairwise different, single particle states $\psi_1, \dots, \psi_j, \dots, \psi_n$, initially without considering spin effects. Like Heisenberg, he wanted to know how the n -particle state space decomposes under permutations of the electrons. Each electron was (in the stationary case) identified mathematically by its hypothetical "space coordinates" $r_i = (x_i, y_i, z_i) \in \mathbb{R}^3$, where i served as an index to characterize different electrons.

In his first paper on the topic (Wigner 1926), submitted on November 12, 1926, he considered a product of n "eigenfunctions" ψ_1, \dots, ψ_n . Any state ψ_k can be "occupied" by any (the i -th) electron, which was denoted by Wigner by $\psi_k(r_i)$. He then considered permutation states of the form

$$\psi_{\sigma 1}(r_1)\psi_{\sigma 2}(r_2)\dots\psi_{\sigma n}(r_n) =: v_{\sigma},$$

where σ is any permutation of n elements, (the notation v_{σ} is ours). Thus Wigner studied essentially the same subspace $V^{(n)}$ of the n -fold tensor product of $V = \langle \psi_1, \dots, \psi_n \rangle$ as Heisenberg. In his first paper he considered only the special case $n = 3$ and calculated the decomposition of $V^{(3)}$ into irreducible components under permutations "by hand". No wonder, that he found Dirac's symmetric and antisymmetric representations among them and in addition two 2-dimensional "systems".¹⁷ He concluded similar to Heisenberg:

¹⁵For the following passage on Wigner compare (Chayut 2001) and (Mackey 1993).

¹⁶See (Chayut 2001) and Wigner's autobiographical report in (Wigner 1992, 105).

¹⁷The regular representation of S_3 (cf. next footnote), $R_3 \cong V^{(3)}$, decomposes into the trivial representation U , the antisymmetric representation U' (both 1-dimensional) and two copies of the twodimensional irreducible subspace $S_2 := \{(z_1, z_2, z_3) \mid z_1 + z_2 + z_3 = 0\}$ of the natural representation on \mathbb{C}^3 arising from permutations of the basis vectors: $R_3 = U \oplus U' \oplus S_2 \oplus S_2$.

The additional systems are all degenerate, this degeneration is such that it cannot be broken by any perturbation symmetric in the single particles which are assumed to be equivalent. (Wigner 1926, 34)

The state space $V^{(3)}$ was spanned by vectors v_σ identified by permutations $\sigma \in \mathcal{S}_3$. The operation of \mathcal{S}_3 on $V^{(3)}$ was multiplication of permutations (in Wigner's case from the left), just like in the *regular representation*.¹⁸ In this way Wigner hit, at first unknowingly, upon the problem of a decomposition of the regular representation of the symmetric group \mathcal{S}_3 . His approach to the problem made it apparent that, more generally, $V^{(n)}$ was by its very construction just another version of the regular representation of the symmetric group. It had been studied by Frobenius, Schur, Burnside, Young and others in their works on the representation theory of finite groups.¹⁹

When Wigner discussed this question with J. von Neumann, a good friend of his since their common school days at Budapest, his friend immediately recognized what Wigner was doing from a mathematical point of view and explained the problem in terms of a decomposition of the regular representation. Thus Wigner started the second part of his contribution (submitted November 26, 1926) with a general observation which introduced the representation theory of the symmetric group. Noting the rising calculational complexity, when one wanted to extend the results from $n = 3$ to higher cases, he remarked:

There is a well prepared mathematical theory, however, which one can use here, the theory of transformation groups isomorphic to the symmetric group (...), which has been founded at the end of the last century by Frobenius and has been elaborated later by W. Burnside and J. (sic!) Schur, among others. J. von Neumann was so kind to make me aware of these works, and predicted the general result correctly, after I told him the result for the case $n = 3$. (Wigner 1927b, 43)

Therefore Wigner considered it worthwhile introducing the basic facts of the representation theory of the symmetric group to the readers of the *Zeitschrift für Physik*.²⁰ In particular, he explained in his article how one can calculate the dimension $N_{(\lambda)}$ of a representation of \mathcal{S}_n characterized by a partition

¹⁸The *regular representation* R_G of a finite group G is given by the operation of G on the group algebra $\mathbb{C}[G] := \{\sum_h z_h h | z_h \in \mathbb{C}\}$ (summation of h over G) by operation from the left. It contains all finite dimensional irreducible representations of G . More precisely, in each representation of the symmetric group of n elements each irreducible component X appears in the regular representation with multiplicity $\dim X$. Cf. (Fulton/Harris 1991) or any other book on representation theory.

¹⁹See (Hawkins 1972, Hawkins 1974) and the overview in (Hawkins 2000, 373–384).

²⁰For a more recent introduction to the subject, see (Sternberg 1994).

$(\lambda) := (\lambda_1, \dots, \lambda_k)$ of n ,²¹

$$n = \lambda_1 + \lambda_2 + \dots + \lambda_k, \quad \lambda_i \geq \lambda_{i+1}.$$

After Wigner became aware of the decomposition of the regular representation, he could adapt Heisenberg's perturbation argument for spin coupling to the modified context:

In a system with n equal mass points, between which initially there is no exchange of energy, each eigenvalue is $n!$ degenerate (if the corresponding state does not contain equivalent orbits). If one creates an exchange of energy, each eigenvalue splits into several. (Wigner 1927b, 44)

He proposed to calculate the degeneracy of the corresponding term by the dimension $N_{(\lambda)}$ as above. The basic structure for the splitting of energy terms in an atom with n (peripheral) electrons, which had been translated by Heisenberg into the problem of decomposing $V^{(n)}$ into minimal invariant subspaces, was now elucidated by applying standard methods of representation theory for the symmetric group. To Wigner and von Neumann this turn may have appeared like some kind of "pre-established harmony" between physics and mathematics, stipulated in the contemporary Göttingen milieu of mathematics and mathematical physics. For other participants it may have looked more like a kind of magic of mathematical symbolism.

On the other hand, many questions were still open. Among them most importantly the question which of the irreducible representations of the permutation group on the space of Schrödinger wave functions were compatible with the Pauli-Dirac principle of antisymmetry for the total (Pauli-) wave function. In order to address this question, the spin phenomenon and its relation to rotational symmetries had to be understood better.

2. Wigner and von Neumann

Early in 1927, Wigner made considerable advances. He enriched the study of invariance by including rotations of the state space of electrons in an outer atomic shell. In his third paper in spectroscopy, he started to derive the basic structural data of spectroscopic terms from the rotational symmetry of the electron state spaces (Wigner 1927a).²² Already in the introduction to the paper he stated:

The simple form of the Schrödinger differential equation allows us to apply certain group methods, more precisely, representation

²¹The dimension of $N_{(\lambda)}$ is the quotient of $n!$ by the product of all "hook lenghts" of the corresponding Young diagram. For details see (Sternberg 1994, 89ff.).

²²Received May 5, 1927.

theory. These methods have the advantage that by their help one gets results nearly without calculation, which do not only hold *exactly* for the one-particle problem (hydrogen atom), but also for arbitrarily complex systems. The disadvantage of the method is that it does not allow us to derive approximative formulas. In this way it is possible to explain a large part of our qualitative spectroscopical experience. (Wigner 1927a, 53)

Representations of the rotation group

Again it was J. von Neumann who advised Wigner what to read in order to understand the representation theory of the special orthogonal group SO_3 , in particular the recent papers by I. Schur and H. Weyl (Schur 1924, Weyl 1924b).²³ Thus Wigner discussed, among others, the irreducible representations of the rotations in the plane, SO_2 , which are (complex) 1-dimensional. They are characterized by an integer parameter m , such that any plane rotation δ_α by an angle α has the representation as the (one by one) “matrix” e^{ima} . Let us denote, for brevity, this representation of the plane rotation group as d^m . Then, of course, the representation matrix of the rotation δ_α is the 1×1 matrix

$$d^m(\delta_\alpha) = e^{ima};$$

in other words, the representation of the rotation by the angle α has the eigenvalue e^{ima} .

Wigner then introduced the $(2l + 1)$ -dimensional representations of SO_3 (of highest weight $l \in \mathbb{N}_0$), which we denote here as \mathcal{D}^l , according to present conventions, and indicated how to calculate the representation matrices

$$\mathcal{D}^l(A) = (D_{jk}^l(\alpha, \beta, \gamma))_{1 \leq j, k \leq 2l+1}$$

for any rotation $A \in SO_3$, characterized by its three Euler angles α, β, γ (Wigner 1927a, 68ff.). Moreover, he discussed the decomposition of \mathcal{D}^l under restriction to the subgroup SO_2 of rotations about the z -axis into $2l + 1$ one-dimensional subspaces. This leads to representations d^m in our notation above, where m may assume the $2l + 1$ pairwise different values

$$-l \leq m \leq l.$$

That fitted structurally so well with the observed classification of spectra and their discrete parameters, the quantum numbers, that Wigner could immediately proceed to a spectroscopical interpretation of these representation theoretic quantities. The highest weight l could be identified with the *azimuthal quantum number* of the Bohr-Sommerfeld theory (Wigner 1927a,

²³See (Wigner 1927a, 63, fn. (1)).

71) (later often called *orbital angular momentum* quantum number).²⁴ Moreover, the weight m of the specified abelian subgroup SO_2 appeared as a group theoretic characterization of the *magnetic quantum number* of the electron. The latter had been introduced in order to explain the split of spectral lines (indexed by the *principal* quantum number n of the so-called Balmer-series and by l) into different terms (“multiplets”) under the influence of a strong magnetic field, the so-called normal *Zeeman effect*.²⁵ A similar effect had been observed under the influence of a homogeneous electric field (*Stark effect*).²⁶ Thus the basic features of the dynamics of the electron were apparently closely related to the basic parameters of representations of the symmetry group of its orbit.

After a short discussion of the fact that transitions of electrons occurred in nature only between neighbouring azimuthal (orbital angular momentum) quantum numbers l , corresponding to a change $\Delta l = \pm 1$, Wigner turned to the consequences of the introduction of a homogeneous electric field:

By means of an electric field along the Z -axis the substitution group of our differential equation is diminished (verkleinert). Thus we have to proceed [as above] and reduce the three-dimensional rotation group to a collection of representations of the two-dimensional group (about the Z -axis). (Wigner 1927a, 72)

As a result, under the influence of an external homogeneous field, a term with azimuthal quantum number l splits into $2l + 1$ lines, indexed by the magnetic quantum number m .²⁷

For atoms with more than one electron involved in radiation processes, the situation was, of course, much more complicated. Here Wigner could only vaguely indicate, how the representation of the rotation group and of permutations might work together to form the total state space of an n -electron system and how they determine the combined quantum numbers (Wigner 1927a, 77f.).

The spin group SU_3

For a detailed investigation, a more subtle study of the interplay between rotational symmetry, its relation to spin properties, and the exchange symmetries (permutations) of multi-particle systems became necessary. At almost

²⁴In spectroscopy, an alphabetical code is used for l : S for $l = 0$, P for $l = 1$, D for $l = 2$ etc..

²⁵With a magnetic field in direction of the observation, P. Zeeman had observed such an effect in 1896, while perpendicular to the field a “third” (undisplaced) line appeared. H.A. Lorentz had explained it a year later in terms of a classic theory of the electron in the magnetic field, cf. (Rechenberg 1995, 161), (Darrigol 2001) or (Pais 1986, 76f., 268ff.).

²⁶The Stark effect had been observed in 1913.

²⁷In this context (Stark effect), Wigner called m the “electric quantum number” (Wigner 1927a, 73).

the same time as Wigner's paper on rotational symmetries, Pauli submitted his path-breaking proposal to mathematize Uhlenbeck's and Goudsmit's hypothesis of an intrinsic "spin" of the electron by the use of "two-component" wave functions (Pauli 1927).²⁸ Charles G. Darwin stepped in with a series of papers on the "electron as a vector wave".²⁹ That made it possible for Wigner to extend the investigations of symmetries to spin effects.

For such studies von Neumann's advice became even more important than before. The publications discussed above were written by E. Wigner when he was still an assistant for theoretical chemistry at the technical university Berlin. In spring 1927 he moved to Göttingen for one year, as an assistant of Hilbert's. At that time, Hilbert suffered strongly from pernicious anemia and was nearly inaccessible to his new assistant. Nevertheless, Wigner came into close contact with other young physicists working at Göttingen, among them in particular L. Northeim, P. Jordan, and W. Heitler. Moreover, von Neumann visited Göttingen regularly (Mehra 1993). Thus there were good conditions for Wigner and von Neumann to establish the basic representation theoretic features of atomic spectra, including spin effects, during late 1927 and the first half of 1928, simultaneously with H. Weyl's work on the same topic and independently of it.

Between December 1927 and June 1928, E. Wigner and von Neumann submitted a series of three papers on spectra and the "quantum mechanics of the spinning electron (Drehelektron)" to the *Zeitschrift für Physik*.³⁰ As Wigner later reported, he wrote the papers after intense discussions with his colleague and friend whom he therefore considered to be a coauthor (Mehra/Rechenberg 2000/2001, 496). In this series, the authors emphasized the conceptual role of representation theory for quantum mechanics in an explicit and programmatic manner and parallelized it to the invariance method of general relativity.

... It may not be idle to call the strong heuristical value (Spürkraft) to attention, which dwells in these and similar principles of symmetry, i.e. invariance, in the search for the laws of nature: In our case it will lead us, in a unique and compelling way, from Pauli's qualitative picture of the spinning electron to the regularities of the atomic spectra. That is similar to the general theory of relativity, where an invariance principle made it possible to unveil the universal laws of nature. (Wigner/v.Neumann 1928a, 92)

In their paper, Wigner and von Neumann took up Pauli's characterization of spin by a (commutative) product of a Schrödinger wave function

$$\psi(x), \quad x = (x_1, x_2, x_3) \in \mathbb{R}^3,$$

²⁸Received May 8, 1927, by *Physikalische Zeitschrift*, three days after the submission of Wigner's paper (Wigner 1927a).

²⁹(Darwin 1927, Darwin 1928)

³⁰Dates of reception: December 28, 1927; March 2, 1928; June 19, 1928.

and a complex function $\zeta(s)$ depending on variable in a discrete two-point “internal” spin space, $s \in \{\pm 1\}$. The combined function

$$\varphi(x, s) = \psi(x)\zeta(s) \quad (3)$$

had been introduced by as Pauli as (spin-) wave function. The dependence on s could just as well be written in index form

$$\varphi_s(x) := \varphi(x, s), \quad \text{with } s \in \{\pm 1\}.$$

Then the Pauli wave function was given by two components,

$$\tilde{\varphi}(x) := (\varphi_{-1}(x), \varphi_1(x)),$$

and $\tilde{\varphi}$ could be considered as a modified wave function (on \mathbb{R}^3) with values in \mathbb{C}^2 , a “hyperfunction” in Wigner’s terminology (later called a *Pauli spinor field* on \mathbb{R}^3).

For an n -particle system the wave function acquired the form

$$\tilde{\varphi}(x_1, \dots, x_n) := (\varphi_{s_1 \dots s_n}(x_1, \dots, x_n)), \quad x_j \in \mathbb{R}^3, s_j \in \{\pm 1\}. \quad (4)$$

Then the values of $\tilde{\varphi}$ were in \mathbb{C}^{2n} (Wigner/v.Neumann 1928a, 94)

Wigner and von Neumann studied how to express the operation of the rotation group SO_3 on the Pauli wave-functions by a unitary operator. They introduced an explicit expression for the complexified version \tilde{A} of a rotation $A = A(\alpha, \beta, \gamma)$ given in terms of the Euler angles α, β, γ (Wigner/v.Neumann 1928a, 98),

$$\tilde{A} := \begin{pmatrix} e^{-i\frac{\alpha}{2}} & 0 \\ 0 & e^{i\frac{\alpha}{2}} \end{pmatrix} \begin{pmatrix} \cos \frac{\beta}{2} & \sin \frac{\beta}{2} \\ -\sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{pmatrix} \begin{pmatrix} e^{-i\frac{\gamma}{2}} & 0 \\ 0 & e^{i\frac{\gamma}{2}} \end{pmatrix}. \quad (5)$$

$$A \mapsto \tilde{A} \in SU_2,$$

such that a rotation $A^{-1} \in SO_3$ operated on the wave-functions by

$$\varphi(x) \mapsto \tilde{A}\varphi(A^{-1}x). \quad (6)$$

That agreed well with what Pauli had done; but while Pauli had made use of the complex description of the spinning top, well known in the Sommerfeld school, Wigner and von Neumann embedded the formula into a representation theoretic perspective. In particular they referred to the second paper of Weyl’s great series on the representation theory of the classical Lie groups (Wigner/v.Neumann 1928a, 98, footnote). Here Weyl had discussed the universal coverings of the special orthogonal groups (later to be

called *spin groups*), had proved the full reducibility and derived the characters and dimensions of all irreducible representations (Weyl 1925/1926).³¹ Von Neumann and Wigner stated clearly that they needed only certain aspects of the general theory.³² But they made quite clear that now one had to take into account “two-valued” representations of the SO_3 , in addition to the (one-valued) ones studied by Wigner in his last paper (called above \mathcal{D}^l , $l \in \mathbb{N}_0$). That gave an additional series which will be denoted here by $\mathcal{D}^{\frac{k}{2}}$ ($\dim(\mathcal{D}^{\frac{k}{2}}) = k + 1$), k odd, according to more recent conventions.³³

For the goal of their paper, they considered the most basic two-valued representation, in fact a local inverse of the covering map

$$SU_2 \longrightarrow SO_3,$$

given by equation (5) up to sign. Then $\mathcal{D}^{\frac{1}{2}}$ was given by the standard representation of the covering group SU_2 ; more precisely

$$\mathcal{D}^{\frac{1}{2}} A = \pm \tilde{A}.$$

In the perspective of their paper, this representation arose naturally from the operation of SO_3 on the 1-particle state as described in equation (6). It was essential to find the consequences for the n -particle state.

They indicated how to find the matrix expressions of a representation matrix $\mathcal{D}^{\frac{k}{2}} A$ for a rotation $A \in SO_3$, characterized by its Euler angles α, β, γ , in analogy to Wigner’s formulas in the classical (one-valued) case. In doing so, they relied on Weyl’s result and stated that for each dimension $n \in \mathbb{N}$ there exists exactly one representation of SO_3 (or its universal cover) indexed by $j := \frac{n-1}{2}$. In the sequel we use the slightly more recent unifying notation for the two series:

$$\mathcal{D}^j = \mathcal{D}^{(j,0)}, \quad \text{of dimension } n = 2j + 1, \quad j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots\} \quad (7)$$

Here n odd (respectively j integer valued) corresponds to one-valued representations, and n even (j half-integer) to “two-valued” representations of the orthogonal group.

With the machinery of representation theory at their disposal, it was clear how to proceed to the description of the n -particle states described by n -fold tensor products. They ended the first paper of the series with an observation on how to decompose the tensor product spaces into irreducible components:

³¹See (Hawkins 2000).

³²“Of course, much less than Weyl’s deep rooted results are necessary for our present goals.” (Wigner/v.Neumann 1928a, 98, footnote)

³³Cf. (Sternberg 1994, 181ff.).

In the applications it will be important to know the irreducible representations of the rotation group in $\{{}^n a_{s,t}^{(\mathcal{R})}\}$ [Wigner/von Neumann's symbol for $\otimes^n \mathcal{D}^{\frac{1}{2}}$, E.S.]; that is easily achieved, as its trace is additively composed from the traces of the former.
(Wigner/v.Neumann 1928a, 108)

They gave an explicit result, described verbally, but without any ambiguity. Written in more recent symbolism, it was

$$\otimes^n \mathcal{D}^{\frac{1}{2}} = \mathcal{D}^{\frac{n}{2}} \oplus (n-1)\mathcal{D}^{\frac{n-2}{2}} \oplus \frac{n}{2}(n-3)\mathcal{D}^{\frac{n-4}{2}} \oplus \dots . \quad (8)$$

Permutations, spin, and anomalous Zeeman effect

In the second paper of their series, Wigner and von Neumann combined the rotational and spin symmetries with the permutation aspect from which Wigner had started. Wigner's basic physical intuition was that in atomic spectroscopy the energy operator H will be composed,

$$H = H_1 + H_2,$$

by a part H_1 resulting from the spatial motion of the electron only (the motion of the "center of gravity" of the electron, as he said) and the ensuing gross effect of the electromagnetic interaction with the field of the atomic core. The second part, H_2 , should model other aspects, most important among them the electron spin (Wigner/v. Neumann 1928b, 133). Thus one could start from the eigenvalue problem of the "spin-less" wave function ψ (Schrödinger wave function),

$$H_1\psi = \lambda\psi ,$$

and refine the result by passing to the "hyperfunctions" φ including spin (i.e., the Pauli spinors).

For the investigation of symmetry properties with respect to permutations, it was therefore natural to distinguish different types of operations for a permutation $\alpha \in S_n$, an operation P on *space variables only* and an operation O on *both*, spin and space variables (P_α and O_α in Wigner's notation):

$$\begin{aligned} P_\alpha^{-1}\varphi(x_1, \dots, x_n; s_1, \dots, s_n) &:= \varphi(x_{\alpha_1}, \dots, x_{\alpha_n}; s_1, \dots, s_n) \\ O_\alpha^{-1}\varphi(x_1, \dots, x_n; s_1, \dots, s_n) &:= \varphi(x_{\alpha_1}, \dots, x_{\alpha_n}; s_{\alpha_1}, \dots, s_{\alpha_n}). \end{aligned}$$

The operation Q of permutations on *spin variables only* could be constructed from these (Wigner/v. Neumann 1928b, 133) by

$$Q_\alpha := P_\alpha^{-1}O_\alpha.$$

Obviously "spin-less" wave functions transformed under P_α , while the transformation O_α of "hyperfunctions" could be built from P and Q , $O_\alpha = P_\alpha Q_\alpha$.

Wigner then considered a slow continuous change from an energy state in which the spin contribution could be neglected ($H = H_1$) to one, in which this was no longer the case (Wigner/v. Neumann 1928b, 133). He made the following observation:

While the original state with $H = H_1$ is invariant under O and P , an increasing spin perturbation H_2 may reduce the original symmetry to O only. In this case, the formerly irreducible subspaces for H_1 are decomposed into smaller irreducible components of $H_1 + H_2$.

That was a convincing group theoretic view of the split of spectral terms by a perturbation bringing spin differences into the game. Empirically such a phenomenon had been observed long ago in the *anomalous Zeeman effect*: If a weak magnetic field was switched on, spectral lines belonging to the same magnetic number m could split into different terms.³⁴

But it was still to clarify how to deal with the antisymmetry principle for the total wave function of an n -electron system. According to Dirac “...only those states occur in nature, the eigenfunctions of which are anti-symmetric” (Wigner/v. Neumann 1928b, 133). Wigner and von Neumann therefore continued with the study of the irreducible representations of the symmetric group \mathcal{S}_n in the antisymmetric part of the total “hyperfunction” representation, i.e., in

$$\wedge^n \tilde{V} \subset \otimes^n \tilde{V},$$

where \tilde{V} denotes a state space of single-particle “hyper-functions” (Pauli-spinor fields). Of course, such irreducible antisymmetric representations are one-dimensional, and the question was, under which conditions such antisymmetric representations in the “hyperfunction” space could be derived from an irreducible representation of the spin-free wave functions. To simplify language, we denote the representation of \mathcal{S}_n in $V^{(n)}$ corresponding to a partition $(\lambda) = (\lambda_1, \dots, \lambda_k)$ by $V_{(\lambda)}^{(n)}$.

If one starts from a degenerate energy term with multiplicity m of the spin-less Schrödinger equation of an n -electron system

$$H_1 \psi = E_0 \psi , \tag{9}$$

one can form a basis of $m 2^n$ corresponding “hyperfunctions”, by allowing for the combinatorics of possible spin values for the n constituents. If analogously m denotes the dimension of an irreducible representation $V_{(\lambda)}^{(n)}$ like above, the $m 2^n$ -dimensional space of spin extended hyperfunctions may be called $\tilde{V}_{(\lambda)}^{(n)}$. Obviously it forms an invariant subspace of $\otimes^n \tilde{V}$ (under permutations). Our authors now looked for irreducible components of $\tilde{V}_{(\lambda)}^{(n)}$, and in particular one-dimensional antisymmetric ones.

³⁴The “anomalous Zeeman effect” had been observed by A.A. Michelson and T. Preston in 1898, and could not be explained in the Bohr-Sommerfeld theory of the atom; cf (Rechenberg 1995, 161f.) or (Pais 1986).

Using a result of A. Speiser's book on group theory (Speiser 1923), they came to the conclusion that a partition (λ) allows to form a (non-trivial, one-dimensional) antisymmetric extension in $\tilde{V}_{(\lambda)}^{(n)}$, if and only if (λ) is of the form

$$(\lambda) = (2, 2, \dots, 2, 1, 1, \dots, 1). \quad (10)$$

That was an important result for the group theoretical program in spectroscopy. It showed clearly, *why (and under which conditions) irreducible representations of the symmetric group could characterize a term system* of higher atoms.

Still the question had to be answered, in how many fine structure terms a spectral line of an n -electron system, corresponding to an azimuthal (orbital momentum) quantum number l and partition (λ) , could split. Thus Wigner and von Neumann finally studied the combinatorical possibilities, by which the total magnetic quantum number $m = m_1 + \dots + m_n$ of such a system could be built from the quantum numbers m_j of the individual electrons and which effects could be expected from switching on a spin perturbations H_2 . They came to the conclusion that the momentum (including spin) of an n -electron system in such a state can be characterized by a (integer or half-integer) value j , called *internal quantum number*, with

$$\left| \frac{n - 2z}{2} - l \right| \leq j \leq \frac{n - 2z}{2} + l$$

(with difference 1 between two values of j). For each j the total magnetic momentum including spin \tilde{m} then may acquire values in $-j \leq \tilde{m} \leq j$. The number t of different values for \tilde{m} , i.e., the number of possible terms into which the n -electron state (λ) with azimuthal quantum number l could split, was then, according to Wigner/v. Neumann (1928b, 140–143):

$$t = \min \begin{cases} n - 2z + 1 \\ 2l + 1 \end{cases}$$

This result agreed beautifully with empirical findings and with the rules derived in other theoretical approaches.³⁵ Wigner was proud about what he had achieved cooperatively with von Neumann:

Thus the, probably, most important qualitative spectroscopical rule has been derived. Independent of the immense effectiveness (Leistungsfähigkeit) of quantum mechanics (...), one will be surprised that all this was “plucked out of the air”, as one might say (daß alles, wie man sagt “durch die Luft” ging), i.e., without taking into account the special form of the Hamiltonian function, only on the basis of symmetry assumptions and of Pauli's qualitative idea. (Wigner/v. Neumann 1928b, 143)

³⁵Like Hund's “Aufbauprinzip” (Wigner/v. Neumann 1928b, 140).

Although definite values of the energy differences could not be derived by group theoretic methods alone, Wigner's and von Neumann's approach gave a convincing explanation for the splitting of a spectral line under a magnetic field (Zeeman effect) of any kind into "multiplett" terms of the fine structure.

3. London and Heitler

In quantum chemistry, representations of permutation groups made their first appearance about the same time as they did in spectroscopy. The topic was opened up by a joint publication of two young physicists, Walter Heitler and Fritz London, who had come to Zürich on Rockefeller grants in 1926 (F. London), respectively 1927 (W. Heitler), to work with E. Schrödinger.³⁶ While a closer scientific cooperation with their professor turned out to be more difficult than expected, they used the opportunity to exchange and develop ideas with each other. In June 1927 they submitted a paper on the quantum mechanical explanation of so-called covalent bonds (those due to valence electron pairs), which arose from an idea of W. Heitler. It soon was considered as the entry point for quantum mechanical model building in chemistry (Heitler/London 1927). According to L. Pauling, one of the great figures of the first generation in quantum chemistry, Heitler's and London's paper can be considered as

... the greatest single contribution to the clarification of the chemist's conception which has been made since G. Lewis's suggestion in 1916 that the chemical bond between two atoms consists of a pair of electrons held jointly by two atoms (Pauling 1935, 340)
(quoted from (Mehra/Rechenberg 2000/2001, 542)).

The story of this invention leads deep into the history of quantum theory and of chemistry and is covered as such in the respective historical literature.³⁷ We want to concentrate here on a specific aspect, which is at the center of our investigation of the use of modern mathematical methods in physical chemistry: the contexts, reasons and mode for the appearance and use of group theoretic methods. Such methods were first applied in two papers by W. Heitler, published in 1928 (Heitler 1928a, Heitler 1928b). They built upon a joint paper with F. London, published during their common summer in Zürich (Heitler/London 1927).

In their joint paper, Heitler and London started from an investigation of two hydrogen atoms and their electrons, initially modelled separately, at a distance $d = \infty$ between the nuclei, by identical Schrödinger functions with energy eigenvalue E_0 . Using a perturbative approach, they studied

³⁶(Gavroglu 1995)

³⁷See (Gavroglu/Simões 1994, Karachalios 2000, Karachalios 2003, Nye 1993, Simões 2003) and (Mehra/Rechenberg 2000/2001, 540ff.).

what happened to the electrons and their added energies when the atomic distance d was reduced. They showed the existence of two solutions, ψ_1 and ψ_2 for the combined system, with respective total energies E_1 and E_2 , and interpreted the energy difference

$$\Delta E_i := E_i - 2E_0 , \quad i = 1, 2,$$

as a kind of *exchange energy* of the electrons.³⁸ With their choice of sign, negative exchange energy expressed that the compound system had a lower energy state than the two single systems. Moreover, the exchange energies were dependent on the distance parameter d . Their analysis showed that, with d increasing from a little above 0 to some value d_1 , E_1 fell to a minimum, rising again for increasing d from d_1 to ∞ , while E_2 fell monotonously for $d > 0$ with increasing d ($d \rightarrow \infty$). Thus ψ_1 represented a bound state for $d = d_1$, while ψ_2 characterized a repulsive force for any value of the atomic distance (the van der Waals repulsion between the two hydrogen atoms)(Heitler/London 1927, 460).

A continuation of the calculation for two helium atoms, each containing two electrons, showed that only the case of a repulsive interaction could be obtained, if electron spin and the Pauli exclusion principle were taken into account (i.e., if both electrons of one atom were assumed to be in different spin states). In this sense, the “exchange energy” of Heitler and London appeared as an effect of spin coupling and was positive in this case. It explained why helium did not form two-atomic molecules and behaved as noble gas. The principles of non-relativistic quantum mechanics seemed to open the possibility of understanding the *structure* (graph-like combinatorics of atomic “valences”) and the *quantity* (energies) of *chemical bonds*.

Heitler's theory of valence bonds

In summer 1928, E. Schrödinger went from Zürich to Berlin, as a successor on M. Planck's chair; in October F. London joined him there as an assistant. W. Heitler, whose Rockefeller grant had run out more or less at the same time, accepted an offer from Max Born to become an assistant at Göttingen. There he got to know E. Wigner whose group theoretic works he had started to read with great interest when in Zürich.³⁹ Now Heitler explored what the representation theory of the symmetric group could achieve for the determination of quantum mechanical bond states.

³⁸The quantum physical idea behind this terminology was the following: If one joined two probability “clouds” about two nuclei to one (of the combined system) some kind of “exchange” of particles between two “partial clouds” related to the nuclei, although fused to represent one state, seemed now possible (i.e., had positive probability). The language of “exchange energy” has to be taken, again, as a classical metaphor for a quantum effect. For a more detailed discussion see (Schweber 1990, 380f.).

³⁹(Mehra/Rechenberg 2000/2001, VI.1, 502, 547)

Already in January 28, 1928, he submitted his first article on the topic (Heitler 1928a). His goal was to extend the approach of his joint work with London to “higher” molecules. For the time being, that did not mean more than two-atomic molecules with $n > 2$ outer electrons. He stated his methodological preferences clearly at the beginning of the paper:

Among all methods, the group theoretic is the one which definitely achieves most for the multi-particle problem: it was brought in by E. Wigner [Heitler referred to (Wigner 1927b, Wigner 1927a), E.S.] to achieve a qualitative overview of all existing terms. (Heitler 1928a, 836)

Heitler came to the conclusion that *already at large distances* the exchange forces between valence electrons of *opposite spin* resulted in a reduction and even a relative minimum of bond energy, which expressed an attractive force between the two atoms. Here he defined *valence electrons* as such electrons of quantum numbers (l, m) in the outer “shell”⁴⁰ which had no partner of equal quantum numbers l, m with opposite spin in the same atom. Heitler hinted at certain restrictions of his approach:

We still have to warn of an overestimation of the implications (Tragweite) of our results in two respects. The simple formulas for the interaction energy ... can only be considered as a very rough approximation, because the perturbative calculation neglects several points and holds only for large distances. Secondly, the “exchange molecules” considered by us represent only a part of the chemical molecules. although of the most prominent and most stable ones (N_2 , O_2 , NH_3 , CH_4 etc.). A large part of the homopolar compounds, however, relies on perturbations of a different kind⁴¹ (Heitler 1928b, 837)

Thus Heitler distinguished clearly between different kinds of chemical bonds only some of which could be explained, in his opinion, by spin coupling accessible to group theoretic methods. He called them *exchange molecules*. We have to keep this in mind when we look at the extension of Heitler’s theory of valence bonds from a more structural, mathematical point of view (e.g., by Weyl) and its reception by physicists and chemists.

Here, Heitler investigated two electron systems A and B , each of which consisted of n (valence) electrons, initially without interaction. All in all, he studied a system of $2n$ electrons. Following Wigner, he characterized a

⁴⁰“Outer shell” now referred to electrons of highest azimuthal (orbital momentum) quantum number l with respect to its spherical symmetry D^l in the atom, and with a compatible magnetic quantum number m ($-2l \leq m \leq 2l$).

⁴¹Heitler referred to the neglection of “polarization” which he estimated for H_2 to be about 25 % and guessed that it should be much higher for higher molecules.

term system by an irreducible representation of the permutation group of $2n$ elements \mathcal{S}_{2n} . Let us call it R .

Under the assumption of no interaction, R could also be considered as a representation of each of the n electrons A and B and thus of two subgroups isomorphic to \mathcal{S}_n , let us say R_A and R_B . The latter were no longer irreducible. Thus Heitler studied the decomposition of R into subspaces which were simultaneously irreducible in R_A and in R_B . This work was facilitated by the assumption (unproved but considered as self-evident by Heitler) that the Pauli principle implies that

... the representations appearing in nature [are] those which contain only 2 and 1 in their partition (Heitler 1928a, 846).⁴²

He concluded that only those representations could appear, in which for both partial systems A and B the respective n valence electrons are characterized by a completely “antisymmetric term system” and have antiparallel spin (Heitler 1928a, 848). On this basis he was able to give an approximative calculation of the exchange energies.

This result established a quantum mechanical explanation of certain non-ionic bonds which could not be explained in terms of Coulomb forces. Traditionally, chemists had used *valence dashes* to represent such molecules. In 1916, G. Lewis had proposed a qualitative interpretation of a valence dash as a pair of electrons shared by two atoms. But the underlying physical forces remained a mystery. Now it seemed promising to look for an explanation of such “valences” by the pairing of electrons with opposite spin, but otherwise equal quantum numbers. Heitler’s proposal was thus to investigate the range of the hypothesis that *spin coupling of valence electron pairs* lay at the base of molecule formation.

In a second article on the topic, submitted September 13, 1928, Heitler extended his investigations to molecules with more than 2 atoms (Heitler 1928b). Here Heitler was less cautious than in January. He now described the result of his first article as having established a “complete equivalence” of the quantum mechanical explanation of homopolar chemical bonds for two-atomic molecules and the traditional explanation of chemical valences by electron pairs (Lewis). He introduced an integral expression J_Q derived by Heisenberg for the exchange energy between two systems Q , constituted by the partial systems A and B (Heisenberg 1928), and resumed:

Each such exchange energy J_Q between two atoms can be interpreted as a *valence bond* symbolically denoted by a valence dash (Valenzstrich). Nearly all typical and stable two-atomic molecules of chemistry rely on such an exchange bond; and vice

⁴²This condition was proved a little later by Wigner in his joint work with von Neumann, as we have seen. It may have been orally communicated knowledge in Göttingen already in winter 1927/28.

versa: if the valence theory permits the existence of a two-atomic molecule then it is possible quantum mechanically. (Heitler 1928*b*, 805, emphasis in original)

Although his theory did not predict new or different effects in comparison to classical chemical knowledge, it claimed to explain the empirical knowledge of valence bonds structurally, for the case of *two-atomic* molecules. Moreover, it should lead to a quantitative determination of bond energies, even if only in the sense of a rough, first estimation (see quotation above).

Other approaches

Competing approaches to the quantum mechanics of chemical bonds were developed by F. Hund and a little later by L. Pauling, R. Mulliken, and others. They shed doubt on the range of Heitler's and London's theory and on its quantitative reliability. They did not rely on the exchange energy of spin coupling, but concentrated on the spatial distribution of the Schrödinger function. During the next decade it turned out that for more complicated molecules Heitler's method led to unrealistic predictions. The alternative approaches were necessary, even on the structural level, to achieve a satisfactory agreement with experimental knowledge.

In summer 1928 these consequences were not yet clear, although chemists like Mulliken and Pauling already thought along different lines.⁴³ For a short while Max Delbrück who became well known for his later researches on the molecular basis of genetics considered Heitler's and London's approach worth following. He studied perturbative formulas for the determination of exchange energies based on group theoretical methods (Delbrück 1928). Thus Heitler could see his position strengthened and contributed to further explorations of his method in (Heitler 1928*b*). Here he posed the fundamental question as to the *existence* of multi-atomic molecules, on the basis of exchange energies of valence pairs of electrons.

This type of question was highly interesting from a mathematical point of view, but may have appeared useless to most chemists. Heitler considered his investigation as nothing more than a "preliminary study (Vorstudie)". In the course of it, he came to admit that in the calculations of exchange energies, it might happen that permutations of more than two electrons contribute essentially to the interaction. That had already been conjectured by F. London. Heitler remarked that, in his opinion, bonds which rely on such higher exchanges could not be considered as "valence bonds in the sense of Lewis". They would constitute a different type of bond. Nevertheless he thought it justified to study, how far one could come with valence bonds proper ("in the sense of Lewis") (Heitler 1928*b*, 815). At the time, he still

⁴³See (Gavroglu/Simões 1994, Nye 1993) or (Mehra/Rechenberg 2000/2001, 552ff.).

hoped that chain molecules of organic chemistry and lattice structures might belong to “our bond category” (Heitler 1928*b*, 806).

This hope did not come true. During the 1930s, L. Pauling’s and R. Mulliken’s approach of constructing “molecular orbitals”, i.e., Schrödinger functions of multi-electron systems about a complex of atoms (molecular core), built much less on structural principles such as permutations. They drew upon previously unformalized chemical knowledge on hypothetical spatial constellations of the atoms for the modelling of Schrödinger functions of a system of electrons. The striking successes of this approach turned out to be crucial for the acceptance of quantum mechanics among chemists (Gavroglu/Simões 1994). It became the core mathematical technique during the next few decades for a fruitful elaboration of quantum mechanical models for more complicated molecules, in particular in organic chemistry.⁴⁴

3. Weyl at the backstage

Taking the results of Wigner, von Neumann, and Heitler into account, it might look as if not much was left for Hermann Weyl when he entered the field. But such an impression would be completely wrong; Weyl took up a whole range of questions pertaining to the challenging new field and entered into second phase of active involvement in mathematical physics between 1927 and 1931. This second phase was a natural follow up to his first phase of activity in theoretical physics between 1917 and 1923, in which he had made crucial contributions to general relativity, unified field theory, and cosmology.⁴⁵ When he entered the terrain of quantum mechanics, he was particularly interested in the role of group representation and contributed to the introduction of gauge methods into the quantum physical setting.

The background of Weyl’s intervention in the field was one of the surprising conjunctions in the history of science, which turned out to be tremendously fruitful. During the years 1925/26 the München-Göttingen-Copenhagen group of Heisenberg, Born, Jordan, and Pauli, closely communicating with Bohr, invented quantum mechanics; Schrödinger, at that time working at Zürich, complemented it with his “wave mechanics”, P.A.M. Dirac, in Cambridge, developed his perspective of “q-numbers” (a formal operator symbolism, particularly well adapted to the physicists way of thinking) and crowned the whole development by an overarching view – called “transformation theory” by physicists.

At the beginning of this period, in April 1925, Weyl had just finished his great work on the representation theory of classical (Lie-) groups.⁴⁶ For him,

⁴⁴Up to our days, it continues to be the basis for the semi-classical approximations used as building blocks for the computer simulations of molecular structures, cf. (Le Bris/Lions 2005).

⁴⁵See (Sigurdsson 1991, Coleman/Korté 2001, Scholz 2001*c*, Mackey 1988, Speiser 1988).

⁴⁶Weyl delivered the three parts of the series (Weyl 1925/1926) in January, February,

it was not only the attraction of the fascinatingly rich mathematical structures of covering groups, decomposition of representations into irreducible spaces, calculation of characters, classification of root systems, weight vectors, and reflection groups etc., which made him turn towards this work, but rather its intriguing interplay with conceptual questions lying at the basis of physical theory building. Weyl had met classical groups and Cartan's classification of their infinitesimal versions (Lie algebras) on two occasions during his first phase of active involvement in mathematical physics. He found them to be crucial for answering two questions in this context:

- Why are tensors such a good and, in fact, universal tool in general relativity and, more general, in differential geometry?
- What are group theoretic reasons for the “pythagorean” (Weyl’s terminology for what later was called semi-Riemannian) nature of the metric in general relativity?

The *first question* was answered by Weyl in 1925 with the insight, and its proof, that all irreducible representations of the general linear group $GL_n\mathbb{R}$ can be constructed as invariant subspaces of tensor powers of the underlying standard representation (for differential geometry, $V = T_p M \cong \mathbb{R}^n$, the tangent space at a point p to the underlying manifold M). In this sense, tensors and tensor spaces were universal objects for the representation of the general linear group. For the proof he could build upon methods developed by I. Schur in his dissertation from 1901, complemented by an idea of Hurwitz (the so-called unitarian restriction) to prove complete reducibility. All the irreducible representations could then be characterized by some *symmetry condition* inside some tensor power $\otimes^k V$. Thus an intriguing correspondence between the representations of the symmetric group S_k and the irreducible representations of $GL_n(\mathbb{R})$ inside $\otimes^k V$ (representations of “order k ”) played an important role in the answer to his first question.⁴⁷ During the next two years, this correspondence turned out to be intimately related to the construction of state spaces for k “indistinguishable particles” (often electrons bound in an atom) from the state spaces of the single particles.

This result appeared all the more important to Weyl, as already *before* the advent of quantum mechanics he had formed the conviction that exactly such irreducible subspaces of $\otimes^n V$ form the proper mathematical domain of the classical physical field quantities. He considered the relativistic electromagnetic field tensor F_j^i with its antisymmetry property ($n = 2$),

$$F_j^i + F_i^j = 0 ,$$

and April 1925. For this part of the story see (Hawkins 2000, Borel 2001, Slodowy 1999).

⁴⁷(Hawkins 2000, 455ff.)

as an outstanding example for this principle. The methods developed in the study of the general linear group became the clue to his general theory of representation of the classical groups.

The *second question* had been answered by Weyl already a little earlier in his investigations of the “mathematical analysis of the problem of space”. It had given him reason to absorb more of E. Cartan’s classification of the infinitesimal Lie groups than before.⁴⁸

During the crucial years 1925 and 1926, Weyl was busy in other fields. Immediately after he had finished his researches in representation theory of Lie groups, he started intense reading for a book-length article on philosophy of mathematics and natural sciences, which he had promised to the editors of a handbook of philosophy.⁴⁹ In winter semester 1926/27 he lectured on the theory of continuous groups and their representation as a guest at the Göttingen mathematical institute.⁵⁰ Nevertheless he was well aware what was going on in quantum mechanics. Even more than that, he actively participated in the internal discourse of the protagonists. He was in regular communication with E. Schrödinger who taught at the university of Zürich in direct neighbourhood to the ETH where Weyl was teaching. And he continued to be a kind of external “corresponding member” of the Göttingen mathematical science milieu – notwithstanding his differences with D. Hilbert on the foundations of mathematics.

Communication with M. Born and P. Jordan

In the fall of 1925, Weyl corresponded with M. Born and P. Jordan on their actual progress in clarifying Heisenberg’s idea of non-commuting “physical quantities” in quantum mechanics, which was initially stated in a mathematically rather incomprehensible form.⁵¹ Heisenberg’s idea was ingenious and opened new perspectives for theoretical physics, but it was very difficult to understand. It became a comprehensible piece of mathematical physics only after the clarification brought about by joint work with Born and Jordan on the one side and by Dirac’s contributions on the other.⁵²

Weyl was well informed about the work done by the Göttingen physicists and even contributed actively to the research discussion among Born, Jordan,

⁴⁸See (Hawkins 2000), (Scholz 2001b, Scholz 2004b). The order of the questions is here given according to their relative importance identified by Tom Hawkins for Weyl’s turn towards the new research project in representation theory of Lie groups.

⁴⁹Published as (Weyl 1927a).

⁵⁰In this lecture Weyl did not yet touch the application of group theory to quantum mechanics (Weyl Ms 1926/27). I thank M. Schneider who found H. Grell’s *Ausarbeitung* of Weyl’s guest lecture in the *Nachlass* Herglotz.

⁵¹(Heisenberg 1925) submitted July 29, 1925.

⁵²The first paper of Born and Jordan (Born/Jordan 1925) was received on September 27, 1925, by the *Physikalische Zeitschrift* and a succeeding one by all the three (Born/Heisenberg/Jordan 1926) on November 16, 1925. Dirac joined on November 5, (date of reception) (Dirac 1925).

and Heisenberg in the crucial months of mid and late 1925. In September 1925 Born visited Weyl at Zürich and reported him about the latest progress in quantum mechanics. Weyl immediately started to “calculate a bit to clarify things” for himself, as he wrote to Jordan a little later.⁵³ He informed Born about his insights with great admiration for the work of the Göttingen physicists:

Dear Herr Born!

Your Ansatz for quantum theory has impressed me tremendously.

I have figured out the mathematical side of it for myself, perhaps it may be useful for your further progress . . . (Weyl Ms1925a)

Weyl proposed to consider the relationship between unitary one-parameter groups $P(\delta)$ and $Q(\epsilon)$ with their anti-hermitean infinitesimal generators p , and q

$$P(\delta) = 1 + \delta p + \dots \quad \text{and} \quad Q(\epsilon) = 1 + \epsilon q + \dots \quad (0 \leq \delta, \epsilon).$$

He argued that the properties of the (Lie) algebra generated by pairs of conjugate infinitesimal operators,

$$pq - qp = \hbar 1,$$

with 1 the identity and “ \hbar a number”, as Weyl wrote (he omitted the imaginary factor i), could be related to a commutation relation among the integral operators like

$$PQ = \alpha QP, \quad \alpha = 1 + \hbar \delta \epsilon + \dots$$

Typical relations among the infinitesimal operators could then be derived from this approach.⁵⁴

About a week after the submission of his joint article with Jordan, Born gave a friendly answer, but with a certain reserve. He wrote:

It was a great pleasure for me to see that our new quantum mechanics attracts your interest. In the meantime, we have made considerable progress and are now sure that our approach covers the most important aspects of the atomic structure. It is very fine (sehr schön) that you have thought about our formulas; we have derived these formulas in our way, even if not as elegant as you, and intend to publish the subject in this form, because your method is difficult for physicists to access. . . (Born Ms 1925)

The communication went on. Weyl received a page proof of the submitted paper directly from the *Zeitschrift für Physik* and wrote a supportive letter

⁵³(Weyl Ms1925b)

⁵⁴As an example Weyl presented the characterization of the formal derivative $f_q := np^m q^{n-1}$ of a monomial $f = p^m q^n$ used by Born and Jordan: $f_q = \hbar^{-1}(pf - fp)$.

to the younger colleague, P. Jordan, in which he apparently referred to his alternative approach to the commutation relations once more.⁵⁵

Jordan thanked Weyl for his comments on November 25, 1925, shortly after submission of the second paper jointly written with Heisenberg. He remarked that he had read Weyl's letter to Born at the time "with great interest". He emphasized that Born and he had come close to a *derivation* of the canonical commutation relation from the definition of the derivative $\frac{d}{dt}A$ of an operator valued function $A = A(t)$ of a real variable t . In a footnote he added:

When Born talked to you, we still believed that $pq - qp = \frac{\hbar}{2\pi i}1$
is an independent *assumption*. (emphasis in original)

Already in this early correspondence with his colleagues, Weyl looked for unitary groups lying at the base of the quantization procedures used by Heisenberg, Born and Jordan. His proposal of his letter to Born was apparently a first step into the direction of using unitary one-parameter groups obeying a weakened commutativity relation (see below, equ. (12)) as a clue to *derive* the Heisenberg relations from basic properties of projective unitary representations.

In two postcards to Jordan, written in late November 1925, Weyl indicated how in his approach an observable $H = H(p, q)$ given in terms of the conjugate observables p and q could be characterized.

I arrive at a characterization of the domain of reasonable functions H by the Ansatz

$$\int \int e^{\xi p + \eta q} \varphi(\xi, \eta) d\xi d\eta,$$

which is less formal than $\sum p^m q^n$. (Weyl Ms1925c)

This was the first indication of what in his publication two years later (Weyl 1927b) became the proposal to use inverse Fourier transforms for quantization, the now so-called Weyl-quantization (equations (14) and (15) below). Born and his assistant Jordan decided, however, that Weyl's approach was too cumbersome for the introduction of the new quantum mechanics to the physics community, and relied on their own approach. The long delayed and selective reception of Weyl's idea shows that Born may have been right

⁵⁵On November 25, 1925, Jordan wrote to Weyl that the latter could "of course keep the proofs". In a footnote he added an excuse: "I do not know, why they [the page proofs, E.S.] have been sent to you in such a complicated and demanding form (umständlich und anspruchsvoller Form). Born and I are innocent of that (sind unschuldig daran)." (Jordan 1925). We can guess that the printer of the *Zeitschrift* had sent the proofs against acknowledgement of receipt, and that Weyl was a bit perplexed by this procedure wondering, perhaps, whether his Göttingen colleagues wanted to make sure their (undisputed) priority.

in this estimation. On the other hand, his decision may have contributed to the long delay for a recognition of Weyl-quantization as a useful approach in mathematical physics.

Abelian ray representations

Weyl came back to his early proposals nearly two years later in his first article dealing with quantum mechanics (Weyl 1927b).⁵⁶ He clearly distinguished between *pure states* and of *mixtures*. Pure states were mathematically represented by eigenvectors (or more precisely by corresponding complex unit rays) of the typical observables which described the defining properties of a particle or dynamical state. Mixtures, on the other hand, were described contextually as composed from pure states in “any mixing ratio” (Weyl 1927b, 97). In this way Weyl indicated that a mixed state might be characterized by a probability measure on the state space, although he did not spell out details. A little later, and originally without knowledge of Weyl’s manuscript, von Neumann proposed to formalize both mixed and pure systems by (positive) hermitian operators A . Pure states were those given by projection operators onto one-dimensional subspaces and mixtures by more general positive hermitian operators (von Neumann 1927, 215ff.).⁵⁷

Weyl’s main point was, however, the discussion of what he considered the “more profound” question of the “essence (Wesen) and the correct definition of canonical variables” (Weyl 1927b, 91) P and Q , satisfying the *canonical* or *Heisenberg commutation* relation:

$$[P, Q] = \frac{\hbar}{i} 1. \quad (11)$$

He proposed to relate any hermitian operator A to the unitary 1-parameter group generated by its skew hermitian relative iA

$$t \mapsto e^{itA}$$

and to consider the quantum mechanical observables from an “integral” point of view, in the sense of the generated 1-parameter groups. That was a conceptual move similar to the one in Weyl’s work on representation theory, where he found intriguing new aspects by passing from the infinitesimal point

⁵⁶Received October 13, 1927.

⁵⁷Von Neumann presented his paper on November 11, 1927, to the *Göttinger Gesellschaft*. In the page proofs he added a reference to Weyl’s paper (von Neumann 1927, 219, footnote) and vice versa (Weyl 1927b, 90, footnote); compare (Mehra/Rechenberg 2000/2001, 431ff.). In later terms, von Neumann’s positive hermitian operator A can be related to a *trace class* operator T by $A = (T^*T)^{\frac{1}{2}}$, where T is of unit trace norm $T_1 = 1$. Here $|T|_1 := Tr T = \sum_k (Tu_k, u_k) = 1$ with respect to any complete orthonormal set $\{u_k\}$. Moreover, the trace of T can be calculated by the sum of the (positive) eigenvalues a_ν of A , $Tr T = \sum_\nu a_\nu$.

of view (the Lie-algebras in later terminology) to the integral perspective (the groups themselves).

Turning the perspective round, he considered a classical state space described by pairs of n conjugate observable quantities (p, q) , such as the spatial displacement q with respect to a frame and its conjugate momentum p . Then the state space could be considered as an abelian group G of two continuous parameters $(t, s) \in \mathbb{R}^2 = G$ (in the case of $n = 1$ pairs). For the quantization it was natural to look at a *unitary ray representation*, i.e. a representation up to multiplication by a complex number of unit norm.

Then it was clear that in the quantum context the commutation relation for the generating 1-parameter groups e^{itP} and e^{isQ} have to be weakened. Commutativity had to hold only up to a unitary factor,

$$e^{isP} e^{itQ} = e^{icst} e^{itQ} e^{isP}, \quad (12)$$

where c is a real constant normalized to $c = 1$ or $c = \hbar$. Let us refer to equation (12) as the *Weyl-commutation* relation for conjugate pairs of 1-parameter groups in unitary projective (quantum) representations.

Weyl showed that for the corresponding skew-hermitian infinitesimal generators iP, iQ the deviation (12) from strict commutativity implies

$$PQ - QP = -ic1,$$

i.e., the Heisenberg commutation rule (11) for a pair of conjugate observables.

Weyl generalized this procedure to n -tuples of pairs of observables $P_1, Q_1, \dots, P_n, Q_n$. Then a representation on quantum rays⁵⁸ allowed to modify the strict commutation relation of an abelian group $(t_1, \dots, t_n, s_1, \dots, s_n) \in G = \mathbb{R}^{2n}$ to slightly deformed Weyl-commutation relations of the form

$$e^{is_\mu P_\mu} e^{it_\nu Q_\nu} = e^{ic\delta_\nu^\mu s_\mu t_\nu} e^{it_\nu Q_\nu} e^{is_\mu P_\mu},$$

with δ_ν^μ the Kronecker delta and $c = 1$, or $c = \hbar$. For the infinitesimal generators that corresponded to a normalized form of the skew symmetric system of coefficients $c_{\mu\nu}$ in the system of relations (Weyl 1927b, 114)

$$P_\mu Q_\nu - Q_\nu P_\mu = -ic_{\mu\nu} 1. \quad (13)$$

That led to intriguing relations for the addition rule for the $2n$ -parameter unitary ray representation. If we use the denotation $(s, t) \in \mathbb{R}^{2n}$ and

$$W_{s,t} := e^{is_1 P_1} e^{is_2 P_2} \dots e^{is_n P_n} e^{it_1 Q_1} \dots e^{it_n Q_n},$$

the addition becomes

$$W_{s+s', t+t'} = e^{-ic\langle s', t' \rangle} W_{s,t} W_{s',t'},$$

⁵⁸“Quantum ray” signifies that from the one-dimensional subspace, the classical projective ray, only the norm 1 representatives play a role in the quantum mechanical context.

where $\langle s', t \rangle := \sum_\nu s'_\nu t_\nu$ and, as above, $c = 1$ or $c = \hbar$. The resulting structure was an *irreducible projective unitary representation of the abelian group $G = \mathbb{R}^{2n}$* ; Weyl called it an “irreducible abelian rotation group operating on a the field of rays (Strahlenkörper) of pure states” (Weyl 1927b, 118). He restricted his investigation to the case of everywhere defined, bounded (skew-) hermitian generators and the resulting unitary transformations and gave a sketchy argument that these were the only irreducible projective representations for each n .

For a serious application to quantum mechanics, the generalization to the case of unbounded operators was, of course, important. It was solved independently by Marshall Stone and von Neumann (Stone 1930, von Neumann 1931). Von Neumann showed, in addition, that the Weyl commutation relations ((12), (13)) characterize irreducible unitary projective representations of continuous abelian groups up to unitary isomorphism.

Weyl quantization

Weyl, on the other hand, continued his article by looking for a procedure which could give operator companions to (classical) physical quantities in a systematic way, i.e., he looked for a systematic approach to *quantization* (Weyl 1927b, 116). If a classical quantity is expressed by a function $f(p, q)$ of the canonical variables p, q ($f \in \mathcal{L}^2 \mathbb{R}^2$ for $n = 1$), he looked at the Fourier transform ξ of f . Then f can be gained back from ξ by

$$f(p, q) = \int e^{i(ps+qt)} \xi(s, t) ds dt, . \quad (14)$$

Weyl proposed to use the analogously formed operator-valued integral

$$F := \int e^{i(Ps+Qt)} \xi(s, t) ds dt = \int \xi W_{s,t} ds dt \quad (15)$$

as the quantum mechanical version of the physical quantity related to f . In case of periodic variables, pairs (p, q) represent elements on the torus $G = T^2 := S^1 \times S^1 \cong \mathbb{R}^2 / \Gamma$, where Γ is the lattice generated by the periods. Then the integration reduces to a summation over integer numbers s and t in \mathbb{Z} , because the Fourier transform ξ lives on the discrete domain $\hat{G} = \mathbb{Z}^2$. Moreover, f is an element of the function algebra on the abelian group $G = \mathbb{R}^2$, or T^2 in case of periodic variables. For a real valued function f , in particular, the corresponding ξ satisfies

$$\xi(-s, -t) = \overline{\xi}(s, t)$$

and leads to a hermitian operator F .

In the methods introduced and used by physicists at the time for the quantization of classical observables, $p \mapsto P$, $q \mapsto Q$, the non-commutativity

of P and Q led to a fundamental difficulty for an observable given as a function $f(p, q)$ of the basic dynamical variables p and q . Already in the simple cases of a polynomial function, it was not clear which operator one should choose for the formal expression $f(P, Q)$. For example for $f(p, q) = p^2q$ one could choose any of P^2Q , PQP or QP^2 , etc.. Weyl's unitary ray representation approach resolved (or avoided) this difficulty from the outset. The operator inverse of the Fourier transform (15) gave a unique and structurally well determined assignment $f \mapsto F$ of hermitian operators to real valued quantities. Weyl was therefore convinced that “our group theoretic approach shows immediately the right way” towards the quantization problem (Weyl 1927b, 117f.).

Of course, the whole approach worked only for non-relativistic mechanical systems in which time is “the only independent variable”, whereas field theory deals with quantities extended over time *and* space, which relate observations and measurements among each other. Weyl considered the independent variables as “projected into the world” by arbitrary conventions in such a manner that the dependence of physical quantities on them could *not* be measured (Weyl 1927b, 124). In this sense, the independent variables played for him the role of some kind of a-priori component in theory construction. They were necessary for the conceptual architecture of the whole symbolic construction, although they were not directly related to observable quantities. In non-relativistic quantum mechanics time was the only “independent variable” left. He added:

If one wants to resolve the criticized omission of the time concept of the old pre-relativistic mechanics, the observable quantities time t and energy E have to be considered as another canonically conjugate pair, as is indicated already by the action principle of classical mechanics. The dynamical law [of the Schrödinger equation, E.S] will then completely disappear. (Weyl 1927b, 127)

He referred to Schrödinger's first attempts to obtain a relativistic theory of the electron in a centrally symmetric field, but neither here, nor in any later publications, did he start to work out this idea of how one might proceed to build a relativistic quantum field theory. A good occasion would have been his contributions to Dirac's electron theory, two years later; but by then he had already accepted that the physicists working on this question – Dirac, Jordan, Heisenberg, and Pauli – had chosen a completely different approach. They developed the method of so-called second quantization, which seemed easier “to access for physicists”, to take up Born's words from his letter of October 2, 1925 to Weyl.

The problems sketched in Weyl's 1927 paper, the method of unitary ray representations of commutative groups, and the ensuing quantization method proposed were soon reconsidered in Weyl's book (Weyl 1928) and made more accessible to an international audience by its English translation

in 1931. The only traces it left on contemporary work was that of von Neumann and Stone, mentioned above. But it turned out to be of long range inspiration. In the next generation, G. Mackey took up Weyl's representation theoretic perspective and developed it into a broader program for the study of *irreducible projective representations* as a starting point for a more structural understanding of quantum physical systems (Mackey 1949).

In the 1960s, Weyl's quantization started to be revitalized. In this decade, the torus case, $G = T^2$, was reconsidered as a special, and the historically earliest, way to introduce a deformed product on the Fourier dual group, $\hat{G} = \mathbb{Z}^2$. For two elements f, h of the function algebra on G with Fourier transforms $\xi = \hat{f}$, $\eta = \hat{h}$, $\xi, \eta \in \hat{G}$, let the Weyl quantization be written as $f \mapsto F$, $h \mapsto H$. Then the composition of the Weyl quantized operators

$$F \cdot H$$

could be transported back to the original functions f, h or their Fourier transforms ξ, η . That led to a *deformed product* depending on a parameter c (typically $c = 1$ or $c = \hbar$),

$$f *_c g, \quad \text{respectively } \xi \hat{*}_c \eta,$$

with properties which attracted a new generation of researchers.⁵⁹

The resulting non-commutative function algebra on the torus T^2 or its Fourier dual $\hat{T}^2 = \mathbb{Z}^2$ became the starting point for the study of the non-commutative torus, one of the first well-known cases of non-commutative geometry. Weyl-quantization turned out to be just one among a larger class of deformation quantization procedures.

Thus Weyl's first paper presented ideas to the public, which he had developed essentially when he was still “at the backstage” of the quantum mechanical scene, as we have called it, turned out to have long range impact in several respects,

- for the study of *irreducible projective representations* (Stone, von Neumann, Mackey e.a.),

⁵⁹For an overview see (Rieffel 1994). Rieffel refers to (Pool 1966) as the first paper in which an explicit description of the deformed product on the Fourier transform functions was given. His claim that already von Neumann had “pointed out that Weyl quantization induces a new product on functions” (Rieffel 1994, 70) seems, however, to be anachronistic. The closest approximation to such a view in von Neumann's paper is, as far as I can see, a reference to the “Gruppenzahlen” at the end of the paper, where the terminology “Gruppenzahlen” refers to functions f on G as elements of the group algebra $\mathbb{C}[G]$ (von Neumann 1931, 229). Such a perspective was also discussed in Weyl's paper (Weyl 1927b, 106) (and there even in more detail). In the abelian case considered here the group algebra is commutative and could at best serve as the starting point for the introduction of the deformed product. Neither von Neumann nor Weyl mentioned the idea that the Weyl-quantized operators might be used to introduce a modified (non-commutative) product of the “Gruppenzahlen” themselves.

- as an inspiration for the search for conceptually founded quantization procedures such as the *Weyl-quantization*, as it was called after the 1960s,
- and finally as one of the sources for a *non-commutative modification* of the torus (Pool, Rieffel e.a.).

At the time of their publication, Weyl's proposals were, however, far too distant from contemporary quantum mechanical research to be taken up in the physics community. For several decades the paper (Weyl 1927*b*) remained a lonely standing monument.

5. Weyl entering the stage

In late 1927, Weyl entered the field of quantum mechanics with full force. He had announced a lecture course on group theory at the Zürich *Eidgenössische Technische Hochschule*, ETH, for winter semester 1927/28. In the summer of this year, both Zürich theoretical physicists accepted calls to other places, E. Schrödinger left the University of Zürich and went to Berlin; P. Debye gave up his chair at the ETH on occasion of a call to Leipzig. Weyl used the opportunity to reorient his lecture course originally announced on group theory only and offered it now as a course on "Group theory and quantum mechanics (Gruppentheorie und Quantenmechanik)", without running the risk of putting off his local colleagues in physics. Now he had a good opportunity to present his views on group theoretical methods in quantum mechanics. His main interest was centered on the intriguing interplay between representations of the orthogonal group SO_3 (and SU_2) and the permutation group, which about the same time Wigner and von Neumann hit upon from their side. Let us remember that in summer or autumn 1927 only Wigner's own papers were published. The joint work with von Neumann was still going, on when Weyl prepared the book manuscript from the lecture notes in the summer semester 1928. In late August the book was finished and given to the publisher. In the sequel we will also use the abbreviation GQM for it (Weyl 1928).⁶⁰

Weyl's contributions to the topic and the joint work by Wigner and von Neumann were developed in parallel and independently of each other, as far as any direct exchange of ideas is concerned. They nevertheless established a common theoretical approach to groups in the quantum mechanical explanation of atomic spectra. This is a good case for a comparative study of how

⁶⁰If not otherwise stated, quotations refer to the first edition of GQM. If possible translations are taken from H.P. Robertson's English version of the second edition; where necessary or advisable (because of meaning affecting shifts) direct translations from the first edition are given by the author (E.S.). The second edition will be quoted by (Weyl 1928, ²1931), the English translation by (Weyl 1931*a*). For a discussion of the book see (Speiser 1988).

Weyl's perspectives as a mathematician with great expertise in group representations influenced his approach to the subject. We can compare it directly with the Wigner – von Neumann “team”, one of them (von Neumann) a brilliant mathematician who had assimilated the new results in representation theory in a speed which later became legendary, the other one a theoretical physicist of admirable mathematical powers.

Two points of the broader story of group theoretical methods in quantum physics have to be mentioned, before we come to the discussion of Weyl's treatment of the interplay of the symmetric and the orthogonal groups in spectroscopy and quantum chemistry. Here we can only mention them in passing, although they deserve closer scrutiny in their own contexts.

General relativistic spinor fields

Exactly at the end of Weyl's course and shortly after it finished, Dirac's two path-breaking papers on the relativistic theory of the electron appeared (Dirac 1928) and found immediate recognition (Kragh 1990). Therefore Weyl's book already contained a chapter on Dirac's theory. Later in the year 1928 and early the next one, Weyl took up Dirac's theory, simplified it from the point of view of group representations and put it into a general relativistic framework. For physical reasons, Dirac worked with a reducible representation of the Lorentz group, now written as $D^{(\frac{1}{2}, \frac{1}{2})}$, whereas Weyl proposed a reduction to irreducible components, characterized by the standard representation of $SL_2\mathbb{C}$ in \mathbb{C}^2 , $D^{(\frac{1}{2}, 0)}$, and/or its conjugate $D^{(0, \frac{1}{2})}$ (“Weyl spinors” versus “Dirac spinors”, in later terminology). Weyl's main goal in a series of papers in the year 1929 was, of course, of a different nature, the adaptation of spinor theory to general relativity. In this enterprise he had again independent parallel workers, V. Fock and D. Ivanenko at Leningrad. Weyl and Fock/Ivanenko built essentially the same core theory, but differed in outlook and details. That is an interesting story in itself, which cannot be told here.⁶¹ Weyl did *not include* this generalized treatment of the Dirac equation in the second edition of the book, but only referred to it in passing at various places (Weyl 1928, ²1931, VII, 195).

In the second edition he changed and extended, the treatment of the special relativistic Dirac equation. In the first edition he discussed a non-relativistic first approach to “second” quantization of the electron and the electromagnetic field (Weyl 1928, §44). At the end of the passage Weyl remarked:

We have thus discovered the correct way to quantize the field equations defining electron waves and matter waves. The exact realization will be the next task of quantum physics; the maintenance of relativistic invariance seems to offer serious difficul-

⁶¹Compare (Vizgin 1994, Goenner 2004, Straumann 2001, Scholz 2001a).

ties. Here again we find that quantum kinematics is not to be restricted by the assumption of Heisenberg's specialized commutation rules. And again it is group theory, which supplies the naturally generalized variant, as is shown by the next section . . . [in which unitary ray representations and the first steps of Weyl-quantization were presented, E.S.]. (Weyl 1928) (Weyl 1928,² 1931, 203)

In summer 1928, he apparently still assumed that his approach to quantization might allow a generalization from the group IR^3 of non-relativistic kinematics to the relativistic case. In the second edition he omitted the second and the last sentences, after in January 1929 Heisenberg and Pauli had made decisive progress in their approach to "second quantization". Weyl still kept the passage on unitary ray representations and to (Weyl-) quantization, but no longer recommended his own approach as a path towards relativistic field quantization. He included two new sections with a discussion of this new and difficult terrain, following Pauli, Heisenberg and Jordan, although now the obstacle of uncontrollable infinities appeared at the horizon (Weyl 1928,² 1931, chap.IV, §§12, 13).

Discrete symmetries

In these new passages Weyl started also to explore the role of discrete symmetries in the context of early relativistic field theory, parity change P , time inversion T , and charge conjugation C . They ended with a remark which struck readers of the next generation as surprising and even "prophetic":

... this means that positive and negative electricity have essentially the same properties in the sense that the laws governing them are invariant under a certain substitution which interchanges the quantum numbers of the electrons with those of the protons [later readers would functionally rephrase the term by "positrons", E.S.]. The dissimilarity of the two kinds of electricity thus seems to hide a secret of Nature which lies yet deeper than the dissimilarity of past and future. (Weyl 1928,² 1931, English, 264)

We cannot take up the thread of the rise and establishment of the discrete symmetries in quantum field theory here; readers interested in this topic may like to have a look at the discussion in (Coleman/Korté 2001, 293) and (Straumann 2001, 141).

6. Weyl on stage

We come back to comparing the different outlooks of Weyl and Wigner/von Neumann on groups in quantum mechanics. Technically, they agreed com-

pletely, as Weyl frankly stated when he wrote the preface to his book in August 1928.⁶² Discussing the role of group representations in quantum mechanics, he observed:

The course of events is so inevitable (*zwangsläufig*) that nearly everything that was still new at the time when I gave the course has been published elsewhere in the meantime, in particular by the work of the colleagues (der Herren) C.G. Darwin, F. London, J. von Neumann and E. Wigner.

He added:

That is different with Dirac's wave equation of the electron, which introduced essential new ideas into the theory during the time when this book was being written. (Weyl 1928, vi)

The reference to F. London, and at other places to W. Heitler, referred to the theory of molecular bonds, which Weyl had approached with the tool kit of representations of the symmetric group, starting from the joint article of Heitler and London.⁶³ Even more than the other authors, Weyl emphasized the structural role group representations for the understanding of quantum physics. He hoped that they would survive future changes of the actual mathematical models of the atomic or molecular systems:

Recently it turned out that group theory is of fundamental importance for quantum mechanics. In this context it reveals the most essential features *whatever the form of the dynamical law may be, i.e., without definite assumptions on the forces which are acting.* (Weyl 1928, 2, emphasis E.S.)

The last remark described quantum mechanics as a theory in development. Weyl considered it to be in an unfinished state. That differed from the credo of the Copenhagen – Göttingen group which argued strongly in favour of having achieved a “completion” of quantum mechanics.⁶⁴ Weyl did *not* share, however, Einstein's opinion that quantum mechanics had to be considered as of only provisional character, as long as its purely stochastic determination was not reduced to a classical field theory lying at its base. Weyl even had welcomed the stochastical character of natural laws well before the birth of the “new” quantum mechanics (Weyl 1920). Of course, he was, well aware of the fundamental problem that quantum mechanics and

⁶²Remember that all three parts of the Wigner/von Neumann series had appeared at that time, the last one in June 1928.

⁶³(Weyl 1928, ²1931, 300, chap. V, endnote 10). Darwin's publications dealt with the spin phenomenon; among them (Darwin 1927, Darwin 1928). It did not involve explicit group theoretic aspects.

⁶⁴Compare the title of volume VI of (Mehra/Rechenberg 1982–2001): “The Completion of Quantum Mechanics 1926 – 1941”.

relativity had established two theories of basic levels of nature, which were conceptually and mathematically far apart. Already during his “backstage period” Weyl had looked for possibilities of reconciliation of relativity theory and quantum physics (see above). In summer 1928, after Dirac’s breakthrough to a first relativistic quantum theory with empirical successes, he expected further changes to come. In such a period, Weyl thought that the assumptions on the “form of the dynamical law” might still be subject to considerable change. The representation theoretical methods, on the other hand, appeared to him as part of a stable core of quantum mechanical knowledge.

This conviction of a deep structural meaning of group representations was the central topic in GQM. Similar to his first book on mathematical physics, *Space - Time - Matter*, Weyl gave a complete introduction to the mathematics of the field and wrote one of the first textbook expositions of quantum mechanics. He started with an introduction to what he called *unitary geometry*, i.e., the theory of Hilbert spaces and the diagonalization of hermitian forms, although essentially restricted to the finite dimensional case (chapter I). He continued with an introduction to quantum mechanics integrating the Schrödinger view of the dynamical law in the non-relativistic case and the Göttingen (Heisenberg-Born-Jordan) point of view of observables represented by hermitian operators and their quantum stochastical interpretation (chapter II). Of course, he emphasized the turn quantum mechanics had taken with respect to classical natural science. Both had in common to be “constructive”.

Natural science is of a constructive character. The concepts with which it deals are not qualities or attributes which can be obtained from the objective world by direct cognition. They can only be determined by an indirect methodology, by observing their reaction with other bodies; their implicit definition is consequently conditioned by definite laws of nature governing reactions. (Weyl 1928, 66)

Classical mechanics was able to assume that such “constructive properties” were attributes of the “things as such (Dingen an sich)”, in the sense of pertaining to them, even if the manipulations necessary to their determination were not undertaken. In quantum physics this was no longer possible. In this point Weyl agreed with N. Bohr.

With quanta we run into a fundamental barrier (Schranke) to this epistemological position of constructive natural science. (ibid., emphasis in original, my translation, ES)

This limitation lay at the basis of Heisenberg’s undeterminacy relation. Weyl accepted it as a fundamental insight, different from Heisenberg’s mathemat-

ical characterization of the commutation relation.⁶⁵

In the third section Weyl introduced the representation theory of finite groups with some general remarks on continuous groups, their characters and their infinitesimal groups (chapter III). The presentation of concrete examples, in particular the orthogonal group, Lorentz group, the special unitary and the symmetric groups were postponed to the later sections on “applications of group theory to quantum mechanics” (chapters IV and V). Chapter IV contained the theory of atomic spectra, Dirac’s electron theory, and his own method of unitary ray representations. The last chapter developed the combined theory of representations of the unitary group and the symmetric group, preparing his approach to the theory of valence bonds (chap. V).

His presentation of atomic spectra (Weyl 1928, 157ff.) relied much more on theoretical arguments and used less explicit calculations of eigenfunctions than Wigner/von Neumann’s. Nevertheless his discussion went as deep into the physics context as Wigner’s. It included, among others, a concise group theoretic discussion of Pauli’s mathematization of spin and of the anomalous Zeeman effect. Weyl apparently wanted to demonstrate the usefulness of the structural view of mathematics for a conceptual understanding in physics.

Pauli spinors from the point of view of representation theory

For the characterization of electron spin Weyl could build upon his observation of 1924, that the special orthogonal groups $SO_n\mathbb{R}$ are not simply connected but possess, for $n > 2$, a two-fold universal covering group (Weyl 1924a). He clearly distinguished “two-valued” and one-valued representations of these groups (Weyl 1925/1926, II, 602ff.). For the introduction of electron spin, he nevertheless preferred the more physical approach of extending Schrödinger wave functions to Pauli spinors. To concentrate ideas, he started with the discussion of alkali spectra, governed by one external electron with a state space called \mathcal{E} :

We deal with a single electron; the wave function depends only on t and the three space coordinates x, y, z . It cannot be a scalar, however, but is a two-component covariant quantity of type $\mathcal{D}_{\frac{1}{2}}$. Then we have $\mathcal{D} = \mathcal{D}_{\frac{1}{2}} \times \mathcal{E}$, and the decomposition of \mathcal{E} into its irreducible components \mathcal{D}_l with the integer azimuthal quantum number l gives the constituents $\mathcal{D}_{\frac{1}{2}} \times \mathcal{D}_l$. Each of those decomposes again into a doublet \mathcal{D}_j with $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2} \dots$ (Weyl 1928, 162)⁶⁶

The observation of the last sentence was an immediate consequence of the decomposition formula for a tensor product of representations of SU_2 ,

⁶⁵Weyl presented Heisenberg’s undeterminacy in a form due to a communication by W. Pauli (Weyl 1928, 67, appendix 1).

⁶⁶Weyl’s \mathcal{D}_j corresponds, of course, to our $\mathcal{D}^{(j,0)}$ of equation (7).

given here in Weyl's notation (Weyl 1928, 166)

$$\mathcal{D}_s \otimes \mathcal{D}_l = \sum_{j=|l-s|}^{l+s} \mathcal{D}_j .$$

As the old theory without spin characterized the terms very well up to small effects, Weyl assumed that the two-component wave functions were well approximated by the “old” Schrödinger wave functions (as did his quantum physical colleagues). The dimension of the function space was now doubled, with a corresponding rise in the degree of degeneracy. He introduced the notation \mathcal{E}_l for an invariant subspace of \mathcal{E} , $\mathcal{E}_l \cong \mathcal{D}_{\frac{1}{2}} \otimes \mathcal{D}_l$ and gave his interpretation of the appearance of spin doublets:

... thus \mathcal{E}_l now possesses all pairs $\psi = (\psi_1, \psi_2)$ as eigenfunctions They obviously form a linear manifold of $2(2l + 1)$ dimensions. But now a small perturbation term will be added to the wave equation, the “spin-perturbation” which couples the components ψ_1, ψ_2 among each other. Thus the former accidental degeneracy is broken, the $2(2l + 1)$ -fold eigenvalue E_l is split into two values of multiplicities $2j + 1$, with $j = l \pm \frac{1}{2}$, just as the representation $\mathcal{D}_{\frac{1}{2}} \times \mathcal{D}_l$ is decomposed into two irreducible constituents. This is the theory of the doublet phenomenon as sketched by W. Pauli. (ibid.)

This was a beautiful demonstration of how representation theoretic structures appeared very naturally in the material of basic quantum mechanics. They were able to elucidate the symbolic constructions and the perturbation arguments introduced by contemporary physicists, including the kind of structural approximation which led from Schrödinger's to the Pauli's wave functions.

In the discussion of the anomalous Zeeman effect, i.e, the split of spectral lines of multiplets under the influence of an external magnetic field, Weyl showed that the representation theoretic view could also lead to quantitative results; he gave a theoretical derivation of the *Landé formula* for the split of spectral terms in an external magnetic field (Weyl 1928, 164ff.).⁶⁷

⁶⁷Landé had determined a characteristic factor g , important for the calculation of the widths of the line split, as $g = \frac{2j+1}{2l+1}$, where l was the old (integer valued) azimuthal quantum number and $j = l \pm \frac{1}{2}$ an ad-hoc modification which could later be interpreted as the “internal” quantum number of the representation $\mathcal{D}^{(j,0)}$, taking spin into account. Weyl derived g in very good approximation from the magnetic momenta of the Pauli-spinors as $g - 1 = \frac{j(j+1) - l(l+1) + \frac{3}{4}}{2j(j+1)}$, which reduces to Landé's formula in the cases $j = l \pm \frac{1}{2}$. Compare (Mehra/Rechenberg 2000/2001, 499).

A physical role for representations of the symmetric group

In his presentation of molecular bonds and its group theoretic background (chap. V), Weyl was apparently intrigued by a structural analogy of the spin-coupling problem of the n -electron system with his general studies of group representations. In both cases, a strong and deep interplay of a continuous group (SO_3 or SU_2 in the spin case, more generally any classical group) with the operation of the symmetric group, or some subgroup (the Weyl-group in the general case), formed the essential core of his analysis. Thus Weyl declared that one of the goals of his lecture course and the book was to give a unified picture of the representation theory of finite and of continuous groups.

Already from the purely mathematical point of view, it no longer seems justified to make such a sharp distinction between finite and continuous groups as is done in the traditional textbooks.
(Weyl 1928, V)

He was very pleased that the study of the spin of an n -particle system relied on what he called at different occasions a *bridge* between the discrete and the continuous group representations (Weyl 1929c). His goal was to make this bridge conceptually as clear as possible, not only to use its consequences in the determination of term systems or in the investigation of chemical bonds. This does not mean that he contented himself with purely structural insights. He rather started to elaborate the representation theory of the symmetric group with the explicit goal to derive calculatory tools. For this purpose he refined the use of Young diagrams and Young tableaus.

In the last respect he made considerable advances after the publication of the book. Several articles on this topic followed during the next year, among it the main research paper (Weyl 1929a) and some expository ones (Weyl 1929b, Weyl 1929d, Weyl 1929c). In these papers Weyl achieved a structural clarity in the study of spin-coupling, comparable to the one he had gained during the years 1925/26 for the representation theory of the classical groups. On the basis of these results he completely rewrote the last part of his book (chapter V) for the second edition (and its English translation). The revised chapter V became the source for a tradition of a long, although slow, trickling down of knowledge and of symbolical tools from the representation theory of the symmetric group to the theory of atomic and molecular spectroscopy (later even to nuclear spectroscopy) and to quantum chemistry.

In these considerations Weyl employed similar methods to those he had developed in his studies of representation theory in 1924/25. Central for both approaches was the association of a *symmetry operator* A to each element a of the group algebra $\mathbb{C}[S_f]$ of the symmetric group S_f , operating on a tensor product space $\bigotimes^f V$. Using Weyl's notation $F = F(k_1, \dots, k_f)$ for a tensor

$F \in \bigotimes^f V$,⁶⁸ the symmetry operator A associated to

$$a = \sum_{s \in S_f} a(s)s \in \mathbb{C}[S_f]$$

was given by:

$$A : F(k_1, \dots, k_f) \mapsto \sum_{s \in S_f} a(s)F(k_{s(1)}, \dots, k_{s(f)}) .$$

Using such symmetry operators, Weyl formulated symmetry conditions for elements in the tensor space $\bigotimes^f V$ and showed that invariant subspaces of the regular representation on $\mathbb{C}[S_f]$ specify invariant subspaces of $GL(V)$ on $\bigotimes^f V$.

Theorem 1 *There is a 1 : 1 correspondence between invariant subspaces of the regular representation of S_f and invariant subspaces of the operation of $GL(V)$ on $\bigotimes^f V$. The same holds for its irreducible building blocks (the corresponding irreducible representations).*

(Weyl 1929a), (Weyl 1931a, 350)

A comparable correspondence had already been used by I. Schur in his dissertation (Schur 1901) and, in a modified form again in (Schur 1927). Weyl gave full credit to these works. Only his method of symmetry operators was new, and he thought it to be of advantage for the clarification of the overall structure of the correspondence. In an exchange of letters, which is only partially preserved, Schur expressed complete consent:

I do not find anything in your interesting paper which I had to object to. I even accept as not illegitimate the gentle criticism which you offer to my publication from the year 1927. I am very glad to see that you emphasize the connection between my old approach from the year 1901 and your elegant formulation. I also give preference to this direct method and would go even a little farther than you on p. 4 of your manuscript. I am not of the opinion that the later method is the more progressive one.
 (Schur Ms.N.d.)⁶⁹

Any representation of S_f is characterized by a character χ , i.e., the complex valued function on S_f , defined by the trace of the corresponding

⁶⁸This notation takes allows to use a shorthand notation for the operations of $\mathbb{C}[S_f]$ on general tensors $F = \sum_j \alpha_j v_1^{(j)} \otimes \dots \otimes v_f^{(j)}$, defined by linear extension of the naturally defined operation on the decomposable tensors $v_1^{(j)} \otimes \dots \otimes v_f^{(j)}$.

⁶⁹Schur's (undated) letter is an answer to a letter by Weyl, which is not preserved. The discussion relates well to (Weyl 1929a). The only point I cannot identify is the reference to the remark "... on p. 4 of your manuscript ...".

representation matrices. For an irreducible representation it is known that $(\chi, \chi) = 1$, with respect to the scalar product in the function space on S_f . In the sequel we shall use the notation $\rho_V(\chi)$ for the irreducible representation of $GL(V)$ in $\bigotimes^f V$, corresponding to χ by this correspondence and Weyl's theorem.⁷⁰ Weyl considered a spin-extension of the underlying vector space of 1-particle states, V ($\dim V = n$), in the sense of Pauli wave functions,

$$W := V \otimes \mathbb{C}^2, \quad \dim W = 2n. \quad (16)$$

In the case of an f -electron system one has to study the irreducible components of the operation of $GL(V)$ induced on the antisymmetric part of the tensor product, $\bigwedge^n W$. The decomposition of $\bigwedge^n W$ according to Weyl's main theorem leads to multiplicities m_χ for the irreducible representations of type $\rho_W(\chi)$, such that

$$\bigwedge^n W = \bigoplus m_\chi \rho_W(\chi) \quad (17)$$

For the calculation of the multiplicities m_χ Weyl established a kind of “duality” (Weyl's terminology) among the representations of the symmetric group.

To any representation ρ_U of S_f in a vector space U there is an induced representation ρ_U^* on the dual space U^* . By contextual reasons, Weyl modified the sign of this induced operation on U^* by the signum function.⁷¹ Then he could use the apparatus of character formulae and found a striking *reciprocity relation* (Weyl's terminology) between the multiplicity of an irreducible representation of the symmetric group and the dimension of its dual representation:

Theorem 2 *The multiplicities m_χ in (17) are equal to the dimensions of the corresponding dual representations χ^* ,*

$$m_\chi = \dim \chi^*,$$

(Weyl 1929a, 187), (Weyl 1931a, 352).

A direct consequence was that $m_\chi = 0$, if the Young diagram corresponding to χ has more than 2 columns.⁷² From a pragmatic point of view, this

⁷⁰Weyl's notation for our $\rho_V(\chi)$ was $\Lambda_n(\chi)$, where $n = \dim V$.

⁷¹If ρ_U corresponds to a character χ , Weyl defined the *dual representation* χ^* as the representation of S_f given by

$$\sigma \mapsto \text{signum}(\sigma) \rho_U^*(\sigma) \quad (\text{Weyl 1929a, 187}).$$

⁷²The signum factor in Weyl's definition of the dual representation implies $\dim \chi^* = 0$ for dual representations with more than 2 rows. The Young diagram of the representation in the dual space U^* is obtained from the diagram in U by transposition. Thus only representations with Young diagrams of 1 or 2 columns have non-vanishing multiplicities in the decomposition of the alternating product (17) (Weyl 1931a, 350, 352, 370).

result stated the same condition for the existence of an antisymmetric spin extension as the one given by Wigner and von Neumann in terms of the partition (λ) (equation (10)). But Weyl considered this insight as more than just a calculational tool. For him it established a kind of *reciprocity law* of undoubtedly *material importance*.

The modification, which is brought about by the existence of spin under neglection of its dynamical effects and by the Pauli exclusion principle, consists in nothing more than in *a transformation of the multiplicity of the term system corresponding to χ from $[m_\chi]$ into $[\dim \chi^*]$* The dynamical effect of spin resolves these *multipletts* in as many components, as given by its multiplicity $[\dim \chi^*]$; moreover it induces weak intercombinations between the different classes of terms. [Notation adapted to ours, emphasis in original, E.S.] (Weyl 1929a, 188)

Spin coupling in general exchange molecules

Weyl even extended the reciprocity theorem to a more general case, $W = V' \otimes V''$. At first glance, this generalization may look like a pure mathematicians game, without connections to the physical context, but Weyl was highly interested in its application to molecular bonds.

He considered two atoms A and B with electron numbers ν' and ν'' and symmetry types given by the irreducible representations $\mathcal{G}_{\chi'}, \mathcal{G}_{\chi''}$ (with characters χ' and χ'' — Weyl's notation). If they form a molecule, the bond would be described by (collective) states of the combined electron system in the tensor product. The mathematically elementary states would then be characterized by the irreducible representations in the product. Weyl generalized Heitler's and London's theory from exchange molecules with electron pairs to the many ($\nu = \nu' + \nu''$) electron case. His generalized reciprocity theorem (Weyl's terminology) contained the clue for analyzing the possible bonding constellation of higher atoms.

In one of his presentations of the result to a wider audience, a published version of talks he gave during his journey through the United States in late 1928 and early 1929, he explained his basic idea:

This reciprocity law governs the fundamental chemical problem of combining two atoms to obtain a molecule The molecule which is obtained by combining the two atoms will be in one of the symmetry states ζ whose corresponding \mathcal{G}_ζ [Weyl's symbol for an irreducible representation of the full permutation group of all $\nu = \nu' + \nu''$ electrons with character ζ , E.S.] appears in $\mathcal{G}_{\chi'} \times \mathcal{G}_{\chi''}$ and the calculation of the associated energy is accomplished with the aid of these characteristics [characters, E.S.]. These circumstances which cannot be represented by a spacial

(sic!) picture, constitute the basis for the understanding of the homopolar bond, the attraction (or repulsion) existing between neutral atoms ... (Weyl 1929a, 290f.)

With respect to the strong conceptual relationship between mathematics and physics, these words may appear similar to those Weyl had written a decade earlier, in the years between 1918 and 1920 when he pursued his program of a geometrically unified field theory. But during the 1920s Weyl had become much more sensitive to empirical questions. At the end of the decade he had the impression that ground was touched in the formerly fathomless search for a mathematization of the basic structures of matter. This new viewpoint seemed incompatible with the earlier hopes for a unified field theory of matter in terms of classical fields, which Weyl now considered to be illusionary.⁷³ The role played in his earlier work in general relativity and unified field by generalized differential geometric structures was now taken over by group representations in Hilbert spaces (“unitary geometry”) and the quantum theory of atoms and their bonds.

While in the early 1920s he still thought in terms of *a-priori* structures supported by strong methodological and ontological speculations, he now only spoke of an “appropriate language” for the expression of the natural “laws”.

The connections between mathematical theory and physical application which are revealed in the work of Wigner, v. Neumann, Heitler, London and the speaker is here closer and more complete than in almost any other field. The theory of groups is the appropriate language for the expression of the general qualitative laws which obtain in the atomic world. (*ibid.*)

In winter 1928/29 Weyl used a journey to the US to bring the gospel of group theory to the scientifically rising country. He gave lectures at Princeton and Berkeley on “Application of group theory to quantum mechanics” (Weyl Ms1929), and published three articles on the topic in North-American journals (Weyl 1929a, Weyl 1929d, Weyl 1929c).⁷⁴ After his move from Zürich to Göttingen in early 1930, he took part in the seminar on the structure of matter, which went back to the Hilbert tradition and was now run by Born. He was thus led to a further elaboration of his method (Weyl 1930, Weyl 1931b). The second of these notes contained an analysis of determinantal methods used by W. Heitler and G. Rumer in their common work presented in the seminar.⁷⁵

Building on his previous analysis, Weyl showed how to express the spin states of an m -electron system formed from the shells of k atoms, with

⁷³ Compare (Scholz 2004a).

⁷⁴ (Weyl 1929a) was published in German in the *Annals of Mathematics*.

⁷⁵ (Heitler 1931)

m_1, \dots, m_k valence electrons each ($m = \sum_1^k m_j$), and the condition that m_0 valences remained free. Admissible spin coupling constellations of the valence electrons could be constructed from alternating products of the eigenfunctions of pairs of electrons from different atoms. After assigning variables x_1, \dots, x_k to each atom and x_0 to represent empty valences, Weyl developed a method to calculate molecular bond energies. The method relied on the *first fundamental theorem of invariant theory* according to which it is possible to express the invariants of any set of vectors $\{x_0, \dots, x_k\} \subset \mathbb{C}^2$ under the operation of $SL_2(\mathbb{C})$ by integer polynomials in the “fundamental invariants” $z_{i,j}$ derived from the vectors by determinants

$$z_{i,j} := \det(x_i, x_j) \quad 0 \leq i, j \leq k .$$

Weyl used the abbreviated notation $z = [x, y]$ (the *fundamental binary invariant*), for any two vectors x and y .

According to Weyl, a “pure valence state” was characterized by a monomial of total order m and order m_j in each component x_j ($0 \leq j \leq k$), formed from binary invariants $[x, y]$.⁷⁶ Eigenstates of the molecule would not be pure valence states but *superpositions* of them, which are eigenstates of the Hamilton H_p operator of the bound and spin perturbed system,

$$H_p = H_0 + \sum H_{\alpha\beta} ,$$

linearized in terms due to the exchange (transposition) of any two of the valence electrons. Here H_0 denotes the Hamilton operator of the electron system without spin coupling. Weyl developed a method for a calculation of the perturbation term $H_p - H_0$, if the exchange energies $W_{\alpha\beta}$ between two valence electrons ($1 \leq \alpha \leq m_i$, $1 \leq \beta \leq m_j$) of two atoms with index i and j could be calculated (Weyl 1931b, 323f.). The critical point for applications of the method was then the calculation of all the “exchange energies” involved. It presupposed the solution of a generalized version of Heitler’s and London’s problem for electron pairs. Moreover, the whole method could be physically relevant only for molecules for which the exchange energy contributes essentially to the total bond energy. Molecules with large H_0 , with respect to the spin perturbation, could be analysed just as well by studying only the Schrödinger wave component of their Pauli spinors.⁷⁷

From a theoretical perspective, the structure of the procedure was very satisfying. Weyl argued that, by assigning formally a “valence dash” (between atom x and y) to each binary invariant of type $[x, y]$, one arrived at graphs for pure valence states, which were in striking agreement with an old

⁷⁶The totality of pure valence states is not algebraically independent, but obeys a relation, given by the “second fundamental theorem of invariant theory”.

⁷⁷These are molecules in which the geometry of “molecular orbits” of valence electrons and the Coulomb potential are the essential determinants of the bond energy.

proposal by J.J. Sylvester. In 1878, Sylvester had proposed, in a purely speculative approach, to express chemical valence relations by binary invariants. Formally his proposal coincided with the algebraic core of Weyl's construction. Now Sylvester's procedure could be understood as an expression of an algebraic structure underlying the determination of bound states in the new quantum mechanical theory of valence bonds. No wonder that Weyl and Heitler were fond of the new quantum chemical underpinning of Sylvester's speculative method.⁷⁸

There remained, of course, several problems. The practical usefulness of the method could be tested only if the exchange energies of single electron pairs could somehow be calculated. Even then it remained to be seen, whether the result would be in agreement with empirical chemical knowledge. In his first publication, Weyl only indicated the general method (Weyl 1931b, 323f.).⁷⁹ In the 1930s he continued with the calculation of examples. That is shown by notes in his *Nachlass* (Weyl Ms.N.d.) and by remarks in a new appendix written for (Weyl 1949).

But the method was never adopted in the chemical community. Most of the molecules of organic chemistry turned out to be different from the bonding class which Heitler had called exchange molecules, even in Weyl's generalization. During the years, chemists found overwhelming evidence that their models of molecular orbits, in which the spatial distribution of the Schrödinger part of the wave function contributed decisively to the binding energy and sufficed in most cases to solve their problems. Moreover, the method of molecular orbits was closer to the imagination of the chemists and its mathematics was easier to handle for them. The more structural method of exchange energies of spin coupling remained marginal for the practice of physical chemistry, even in the extended and refined form which Weyl had started to develop and to present as a methodological tool to the community of physicists and physical chemists .

7. Outlook

In spite of its surprising theoretical achievements, the rise of groups in quantum mechanics was far from a straight forward story. With its first successes at the turn to the 1930s, there arose sceptical reservation, criticism, and even strong counterforces to the spread of group theoretic methods in the new field of theoretical physics. Such criticism was not always meant as a real opposition to the modernizing tendency; sometimes it was just an expression of uneasiness with the new algebraic methods. Soon after Pauli moved

⁷⁸For a more detailed discussion see (Parshall 1997) and (Karachalios 2003, section 3.1, 163–177).

⁷⁹A graphical method for the construction of a basis of invariants, based on an idea of G. Rumer, was written down by Rumer, Teller and Weyl in (Rumer e.a. 1932).

from Hamburg to Zürich as the successor of Debye, in April 1928, Ehrenfest asked him for help in the difficult new matter. Pauli was well-known for his ability to absorb new mathematics with ease and to adapt it to the necessities of theoretical physics. Moreover, in his last year at Hamburg he had participated in a lecture course on algebra and group theory given by Emil Artin. After his arrival in Zürich in early 1928, he stood once again in close communication with Weyl like in the early 1920s.⁸⁰

Group pest

In September 1928, Ehrenfest turned to Pauli and asked for help in understanding the “terribly many papers on the group-pest (Gruppenpest)”, of which he “could not read any one beyond the first page”, as he wrote to Pauli on September 22, 1928.⁸¹ In parts of the — still small — community, this word became the catchword for opposition to the use of group theoretic methods in quantum mechanics. Apparently Ehrenfest unwillingly contributed a verbal battle sign to the emerging anti-group camp. For him the word expressed nothing more than uneasiness about the rising challenges of the new mathematical methods in theoretical physics. He was not at all opposed by principle to the new tendencies. On the contrary, he supported its development actively. On his initiative, B. L. van der Waerden started to develop his calculus of spinor representations of the Lorentz group (van der Waerden 1929); and one of his later doctoral students, H. Casimir, started to do research work on quantum mechanics, very much influenced by Weyl’s book. As has been discussed on other occasions,⁸² Casimir finally even contributed to the refinement of representation theory itself, by proposing an idea for a purely algebraic proof of the full reducibility of representations of Lie groups, derived from his research on the problem of rotation in quantum mechanics.

Real and strong opposition to the group theoretic approach to quantum mechanics came from another camp led by John Slater, who showed that already traditional algebraic tools were highly effective in the calculation of the energy of higher atoms and binding energies of molecules (Slater 1929). Slater’s background in a more pragmatic tradition of theoretical physics in the United States surely played a role for his strong rejection of the more theoretically minded approaches like representation theory (Schweber 1990).⁸³

⁸⁰(Meyenn 1987), (Mehra/Rechenberg 2000/2001, 472). A couple of weeks after his arrival Zürich, Pauli wrote in a letter to N. Bohr : “I have now learned so much erudite group theory from Weyl that I am really able to understand the papers of Wigner and Heitler” (Pauli 1928). Moreover, he read and commented page proofs of Weyl’s GQM in early summer 1928 (Pauli 1955, 402).

⁸¹Quoted from (Mehra/Rechenberg 2000/2001, 473).

⁸²(Meyenn 1989), (Mehra/Rechenberg 2000/2001, 512–514), (Hawkins 2000).

⁸³See also (Sigurdsson 1991), (Mehra/Rechenberg 2000/2001, 499ff.) and for a broader comparative discussion of German and American physical chemists of the first generation

Slater's success in developing determinant methods for quantum mechanical calculations found immediate acceptance among leading protagonists of the Göttingen milieu. Shortly before Weyl decided to come back to Göttingen as the successor to David Hilbert, Max Born warned him, in an otherwise very friendly welcome letter, that he supported the “attempt to throw group theory out of the theory of atomic and molecular structures, as far as possible” (Born Ms 1930a). At that time, Born was close to finishing an article in which he attempted to get rid of group theoretic methods in the theory of chemical bonds (Born 1930). He even was proud of having convinced Heitler, after the latter's arrival at Göttingen as Born's assistant, to give up the idea that group theoretic considerations might play an important role in studies of molecular bonds.⁸⁴ This perspective resulted in a common article by W. Heitler and G. Rumer on chemical bonds, which only used “traditional” algebraic methods along the line of Slater and Born (Heitler 1931).⁸⁵ On the other hand, group theoretic methods in physics and quantum chemistry continued to be a topic for lecture courses at the Göttingen mathematical institute.⁸⁶

Weyl at Göttingen

In the meantime, in May 1930, Weyl had accepted the call to Göttingen and started to teach there in winter semester of the same year. That gave him a splendid occasion for critical exchanges and collaboration with Born, Heitler, Rumer, and Teller on group theoretical methods in the nascent quantum chemical context. Although Born had been highly sceptical of the method earlier on, he gave critical support to the enterprise after Weyl moved to Göttingen, in his own way. This exchange of ideas with the theoretical physicists around Born in the common Göttingen seminar led Weyl to a more detailed elaboration of his use of symmetry operators in the n -fold tensor space of electron states for the characterization of molecular bond states and the establishment of the link to binary invariants (Weyl 1930, Weyl 1931b). In a subsequent review article on the quantum theory of molecular bonds in the *Ergebnisse der exakten Naturwissenschaften*, Born finally rephrased those results of Weyl's investigation which seemed of importance to him for physicists and physical chemists. In the introduction to his article he frankly declared that the proofs of Weyl's results could not be rephrased under “complete avoidance of the ‘group pest’ which Slater and the author

(Gavroglu/Simóes 1994).

⁸⁴(Born Ms 1930a)

⁸⁵The article was written after Weyl had arrived at Göttingen, and after a discussion of the method in the common seminar on the structure of matter.

⁸⁶W. Heitler gave a course on this subject in winter semester 1929/30 at the mathematical institute (Heitler Ms 1929/30). He concentrated on the subject matter of Wigner's and von Neumann's theory. Only in the last chapter he gave a short introduction to the theory of molecular bonds. I owe Martina Schneider the information on this course.

[Born] had intended". He therefore restricted the presentation to formulas and rules, without proofs, such that the results could be understood by physicists and chemists without being forced to read "the difficult works of Frobenius and Schur on the representation theory of groups", as he wrote in his introduction (Born 1931, 390).

All in all, the first wave of rapid development of group theoretical methods in quantum mechanics ran into the opposition of a strong, multi-faceted, anti-group camp; or, at least, it had to face pragmatic scepticism among physicists and theoretical chemists at the turn to the 1930s.

On the other hand, new forces joined the party of mathematical contributors to representation theoretic methods for mathematical physics. Most important, from the side of young mathematicians, was Bartel Leendert van der Waerden who entered this scene with his spinor paper written with the explicit goal of serving the physics community (van der Waerden 1929).⁸⁷ In personal communications with Weyl he also contributed critical remarks to the understanding of algebraic structures underlying spin coupling. Van der Waerden criticised Weyl's approach from the viewpoint of a young "modern", i.e., structurally oriented, algebraist. In a letter from April 4, 1930, he argued that in Weyl's derivation of the "reciprocity theorem" it was unnecessary to build upon the "inessential property that π [Weyl's symbol for the permutation group, E.S.] is a permutation group". Obviously he abhorred the "multitude of indices" used by Weyl and claimed that one could do without them in this investigation(van der Waerden Ms1930). After some exchanges of letters, of which only the van der Waerden part is preserved, he argued that the result was essentially a question in the representation theory of algebras. According to van der Waerden's analysis, Weyl's result depended essentially on the fact that a matrix algebra \mathcal{A} induced from the operation of the group algebra $\mathbb{C}[S_f]$ on $\bigotimes^f V$ commutes with a completely reducible representation of the general linear group $GL(V)$ on the tensor product (van der Waerden Ms1931).⁸⁸ It seems that Weyl was not completely convinced that such a level of structural abstraction suited his purpose. He rather insisted on the use of the "multitude of indices", because they were essential for the context of modelling the combined electron systems of two atoms in a molecule. Nevertheless he accepted the proposal to straighten the derivation of the reciprocity theorem (Weyl 1931b, 310).

In this sense, the interaction between physicists and mathematicians close to the Göttingen and Zürich milieu seemed to be a splendid scientific environment for a further consolidation of group theoretic methods in physics and chemistry at the turn to the 1930s. In the next couple of years, the triad of now classical text books on the use of group theory in quantum mechanics appeared (Wigner 1931), the second edition of Weyl's GQM and its English

⁸⁷More details will be discussed in (Schneider 2006).

⁸⁸See also (van der Waerden 1930a).

translation by H.P. Robertson (Weyl 1931a), and (van der Waerden 1932). These books broadened the basis for an extension of the approach, invited scepticists to take an own look at the question, and enabled newcomers from different backgrounds to join the enterprise.

From an intermediate period ...

As we know, and most of the participants sensed well, the social stability of this milieu stood on shaky ground. Only little later, with the Nazi's rise to power, the Göttingen mathematical science group was dismantled. As one of the consequences, the closely knit interaction between pragmatic sceptics with respect to the group theoretic method, close to Born, and the group of active protagonists like Weyl, van der Waerden, Heisenberg, Wigner and von Neumann, which was easily organized around Göttingen, was interrupted. Although several of the protagonists of the first wave continued to elaborate and to teach or propagate the new method, no great gains in terms of broader acceptance could be made during the next two decades.

Weyl continued to argue for the use of the new method, in particular in the context of chemical bonds, in publications, talks and lecture courses. But he was very well aware of the reservations of the practitioners of the field felt in regard to his proposals of using invariant theory for the characterization of bond states, and he accepted it. In an undated manuscript of a talk given in the second part of the 1930s, Weyl remarked that the development in the field had not been "very favorable to the scheme" which he had laid out. The recent report (Van Vleck 1935) had nearly passed it over "in silence". He realistically added that in his exposition he even intended to "clearly indicate the boundaries of applicability for our scheme" (Weyl Ms.N.d., 2).

Finally he concentrated his research and publication efforts on the mathematical foundation of the theory. In joint work with Richard Brauer he developed a global characterization of spin representations in any dimension (and of arbitrary signature) by Clifford algebras (Brauer 1935).⁸⁹ All this culminated in his book on *The Classical Groups* (Weyl 1939). That was no disillusioned withdrawal to pure mathematics. It rather was an expression of a realistic evaluation of the actual situation in the field of application. Even though Weyl's calculation of binary invariants did not enter the core of the theory of chemical bonds, his invariant theoretical analysis of spin constellations turned out, in the long run, to be an important contribution to the study of spin-coupling, which has recently started to attract new interest from the point of view of "entangled" systems. The introduction of binary invariants into the study of coupled systems of electrons in the late 1920s and the following decade, may turn out to be another prelude to the

⁸⁹E. Cartan had discussed spinor representations on the infinitesimal level already in 1913; here the integral (global) perspective stood in the center.

development of a symbolic game with long lasting importance in a shifted context of application.⁹⁰

During the decades of slow maturation, it was mainly due to Werner Heisenberg's anticipatory guess of *isospin* SU_2 as a symmetry underlying the nuclear interactions (Heisenberg 1932) and to Eugene Wigner's continuing work and insistence on the importance of the group theoretic approach for fundamental physics, that this research tradition in mathematical physics was never completely interrupted.⁹¹ Most important for relativistic quantum physics was Wigner's fundamental work on the representation theory of the Poincaré group (Wigner 1939).

...to a second wave of groups in quantum physics

With the exception of such “heroic” but for a long time relatively isolated contributions, it needed a new generation of physicists and a diversification of problems and another problem shift in quantum physics, before group theory was stepwise integrated into the core of quantum physics. Faced with the rise in complexity of problems of nuclear spectroscopy, G. Racah brought group theoretic methods closer to the ordinary problem solving practice of spectroscopists (Racah 1942–1949).⁹² Finally the proliferation of new “elementary particles” between 1950 and the 1970s gave material and motivation to look for group theoretical classifications of object structures and the corresponding internal symmetries of interactions. Thus we can see a second wave in the use of group theoretical methods in quantum physics during the 1950s to the 1970/80s. In this changed context, the two books of the above mentioned triad, which formerly were only available in German, were translated into English, (Wigner 1957) and (van der Waerden 1974). Mathematicians of the next generation, among them G. Mackey and I.E. Segal, continued to contribute, from the side of mathematics, to the research tradition begun at the end of the 1920s.

In this second wave of research, simple anticipatory ideas had to be differentiated and different strands of using groups in quantum physics grew together:

- weight systems of representations were turned into a tool for understanding “multipletts” of basic states of matter, generalizing the multiplets of spectral terms of the 1920s,
- isospin was first enriched (“eightfold way”, SU_3) and then transformed into two different forms (weak isospin, SU_2 , and the “chromo-symmetry”

⁹⁰This “game” has recently gained new interest from the point of view of *quantum computing*. In this new context the question of energy contributions, which hindered Weyl's proposals from becoming important in quantum chemistry, are subordinate. I owe the hint to the connection of Weyl's work with these recent developments to P. Littelmann.

⁹¹Cf. (Rasche 1971) and (Mackey 1993, 265f.).

⁹²(Mackey 1993, 269)

- of strong interactions, SU_3), the basic symmetries of particle physics of the late 20th century,
- conservation laws became generally considered as founded upon underlying dynamical symmetries,
 - the study of infinitesimal symmetries became standardized in the form of (generalized and non-abelian) gauge fields or, equivalently, connections in fibre bundles.

Groups, their representations, corresponding conserved quantities, and the use of gauge structures were finally broadly accepted. They were used as an important ingredient of the mathematical forms functioning as a symbolic relative a priori in which theoretical physicists of the late 20th century were able to mold an impressive part of the experimental knowledge of fundamental physics. At the end of the second wave, group theoretical methods were well integrated into the mainstream of mathematical physics. Although at the end of the century the gap between general relativity and quantum physics continued to be wide open, groups and their representations have turned into useful tools and provide conceptually convincing forms for the construction of symbolic models of material processes in both domains.

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